The angular- and crystal-momentum transfer through electron–phonon coupling in silicon and silicon-carbide: similarities and differences

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Abstract
Electron–phonon scattering has been studied for silicon carbide (6H-SiC) with resonant inelastic x-ray scattering at the silicon 2p edge. The observed electron–phonon scattering yields a crystal momentum transfer rate per average phonon in 6H-SiC of 1.8 fs⁻¹ while it is 0.2 fs⁻¹ in crystalline silicon. The angular momentum transfer rate per average phonon for 6H-SiC is 0.1 fs⁻¹, which is much higher than 0.0035 fs⁻¹ obtained for crystalline silicon in a previous study. The higher electron–phonon scattering rates in 6H-SiC are a result of the larger electron localization at the silicon atoms in 6H-SiC as compared to crystalline silicon. While delocalized valence electrons can screen effectively (part of) the electron–phonon interaction, this effect is suppressed for 6H-SiC in comparison to crystalline silicon. Smaller contributions to the difference in electron–phonon scattering rates between 6H-SiC and silicon arise from the lower atomic mass of carbon versus silicon and the difference in local symmetry.

Keywords: electron–phonon scattering, 6H-SiC, RIXS
1. Introduction

For materials properties and function, there is a strong connection between conformation or symmetry on one hand and the electronic structure on the other hand [1]. Therefore, electron–phonon coupling is key to the understanding of these materials. For example, electron–phonon coupling leads to superconductivity following the BCS-theory [2] and the role of electron–phonon coupling on both conventional and unconventional superconductors is the subject of intense research at present [3–8]. As well, the strength of electron–phonon coupling influences the functionality in other materials such as charge-density wave insulators [9], topological insulators [10, 11] and graphene [12, 13] and plays its part in phase changes, such as the Verwey transition in magnetite [14, 15]. In magnetic dynamics, it is apparent that especially the angular momentum (AM) transfer through electron–phonon coupling plays a major role to changes in the spin [16–18]. From the theoretical point of view, when electron–phonon coupling is weak, the separate subsystems of electrons and phonons are relatively well understood [19] and are easily simulated within the Born–Oppenheimer approximation. However, in the strong excitation regime and for a direct dynamical treatment including the electron–phonon coupling, the Born–Oppenheimer approximation fails [20].

This perspective is a major motivation to study fundamental functional materials with experimental techniques. In particular semiconductors like crystalline silicon and silicon carbide (SiC) are important materials. Whereas silicon is the workhorse for information technologies and photovoltaic photon harvesting, SiC is a promising material for high power, high temperature and high frequency applications, because of its extreme thermal and chemical stability together with the large electron saturation velocity and mobility [21, 22] and has applications in light-emitting diodes [21–23], temperature sensors [24] and as neutron detectors [25, 26] and recently intrinsic defects in SiC have been shown to be single-photon sources at room temperature, which is promising for applications in quantum information processing [27, 28]. The most stable of about 100 different polytypes, the hexagonal 6H-SiC, containing six SiC pairs per unit cell and having stacking sequence ABCACB [29] is the subject of this study. The importance of electron–phonon scattering in SiC is illustrated by the fact that SiC light emitters have been developed [22, 23], despite the fact that these materials have an indirect band gap, which generally makes light emission inefficient. It is not exactly known why SiC compounds have such a high efficiency compared to other indirect band gap materials, but one could speculate that the electron–phonon scattering supports fluorescent recombination.

In this work, we determine the electron–phonon scattering rates in 6H-SiC that lead to crystal momentum (CM) transfer and to AM transfer between the scattering subsystems [30, 31]. For this purpose we employ resonant inelastic x-ray scattering (RIXS) at the silicon 2p states, where stringent symmetry selection rules in combination with the femtosecond scattering duration time of RIXS allow to acquire an experimental measure of the crystal and AM transfer electron–phonon scattering rates.

Crystalline silicon was analyzed in a similar study [31]. With the silicon 2p core hole lifetime τ of 8 fs as an ultrafast reference timescale, a temperature-dependent (temperature-independent) CM transfer rate per average phonon of 0.2 (0.4) fs⁻¹ and an temperature-dependent (temperature-independent) AM transfer rate per average phonon of 0.0035 (0.044) fs⁻¹ were determined experimentally through temperature-dependent RIXS. Here, we obtain results for 6H-SiC with the same methodology and compare the results with the previous study on crystalline silicon to extract more general evolutions in electron–phonon scattering.
2. Experimental methods

A 6H-SiC single crystal (0001) as obtained from MaTecK was in thermal contact with a molybdenum plate. The plate was heated either radiatively through a hot filament or with electron bombardment. The temperature of the sample was measured by a pyrometer on the front side, which is at the interaction point with the x-rays.

The spectra were measured with soft x-ray non-resonant and RIXS using our RIXS setup [32] at beamline UE112-PGM1 of the Bessy II synchrotron in Berlin, Germany. The photon energy bandwidth of the beamline was 0.1 eV and the spectrometer had a resolution of 0.2 eV. Si 2p x-ray absorption spectra (XAS) and RIXS spectra using incident x-ray energies at and around the Si 2p edge of 6H-SiC were measured at 25, 300, 600 and 900 °C sample temperature.

The crystal was orientated such that the angle between the incoming x-ray beam and the surface normal was 20° for XAS to avoid self-absorption and 70° for RIXS to maximize count rate. The angle between the incoming x-rays and the RIXS spectrometer was fixed at 90°. The x-ray polarization was horizontal, parallel to the scattering plane. A typical XAS spectrum was measured in 20 min and RIXS spectra were measured in 60 min with an average count rate of 120–200 counts per second.

The intrinsic scattering duration time or the natural lifetime broadening governs RIXS as a resonant Raman scattering process at an inner shell state. The interpretation of RIXS in rate models allows comparing ultrafast dynamic processes to the intrinsic core hole lifetime of the RIXS process [33]. In this study we use the term RIXS for spectra obtained using excitation energies on the XAS resonance or close to the XAS resonance but as well for spectra obtained with excitation energies to the continuum, which is otherwise often referred to as non-resonant x-ray emission or fluorescence.

3. Theoretical section on RIXS

RIXS is a two-photon process and dipole selection rules apply to both transitions [34, 35]. The incoming x-ray photon-excites a dipole transition, in our present Si 2p RIXS study, from a Si 2p core electron to an unoccupied level (either in the conduction band or in the continuum depending on the excitation energy). When this created core hole is filled through a radiative decay from an occupied state, a photon is emitted. The energy and relative number of the emitted photons is measured with the spectrometer.

3.1. AM transfer in RIXS

In the case of Si 2p RIXS, the core hole has a p-symmetric AM state. For the emitted photon in the Si 2p RIXS only transitions from s- and d-electron states to the Si 2p hole are dipole allowed. Nonetheless, p-projected DOS contributions to the RIXS for continuum excitation can sometimes be observed. Although a np → 2p transition is not dipole-allowed since the AM of the photon is not balanced by a change of AM of the electronic states, an effect similar to the observation of d–d transitions in UV–vis spectroscopy is expected to occur: one of the involved states couples with a vibration that balances the AM. In solid systems such a coupling is called electron–phonon scattering. Since in this type of scattering AM of the phonon system is exchanged with the electron system to allow dipole transitions between p-states, the observation...
of p-projected DOS in Si 2p RIXS is a direct measure of the AM transfer due to electron–phonon scattering.

Here we would like to stress that we oversimplify RIXS as a combination of two dipole transitions. It is known that electronic non-dipole transitions can occur in x-ray spectroscopy as was observed and calculated by Jimenez-Mier et al [36]. However, they observed only non-dipole transitions for the higher 3d-transition metal L-edges while they did not observe these non-dipole transitions for the lower 3d-transition metal L-edges. In addition they find that for the higher 3d-transition metal L-edges only 1–5% of the transitions is non-dipole compared to the dipole transition and the non-dipole portion scales with (energy)², meaning that in the intermediate soft x-ray and in the hard x-ray regime the non-dipole contribution becomes stronger. While the Si 2p x-ray edge in the low soft x-ray regime appears at much lower energy than the 3d-transition metal L-edges we can neglect the pure electronic non-dipole transition. Thus, for the present Si 2p x-ray spectra, whenever non-dipole contributions are present in the spectrum, these contributions have to be the result of electron–phonon scattering.

From a direct comparison of the RIXS for continuum excitation with silicon s- and p-projected density of states, the AM transfer can be estimated: for quantitative analysis of the AM transfer, the RIXS spectra for continuum excitation has to be decomposed in s- and p-state contributions using calculations of the silicon s- and p-projected DOS. For this purpose the s-projected calculated DOS was energy aligned to the RIXS based on the main band at 91 eV (this alignment accounts for the relative energetic positions of the screened core-hole and the valence band and is extremely difficult to calculate). The calculated silicon p-projected DOS was shifted with the same energy. For selected regions the integrated areas of the calculated silicon s-projected DOS (DOSₙ), p-projected DOS (DOSₚ) and the integrated areas for the RIXS for continuum excitation (I₉₈₈) at different temperatures were obtained. The regions were selected such that there is one region that in majority contains s-projected DOS, one region that contains in majority p-projected DOS and one region with a combination of s- and p-projected DOS. This increases the accuracy of the analysis.

This quantitative evaluation procedure with the theoretical partial DOS calculated at 0 K assumes that the transition matrix elements in the RIXS are temperature-independent, which is justified through the different energy scales between the RIXS process and thermal excitations [34]. Thermally driven changes of the partial DOS are due to electron–phonon coupling and are the subject of this study. Gathering the values obtained for the three selected regions, an over-determined equation is obtained with three measurements and two unknowns for each temperature, the p-DOS (Fₚ(T)) and s-DOS (Fₛ(T)) fractions in the RIXS spectra. A line is fitted through the acquired data at the different selected regions by I₉₈₈ = DOSₚ × Fₚ + DOSₛ × Fₛ obtaining Fₛ and Fₚ for the different temperatures. From the ratio between Fₛ and Fₚ the relative s-like contribution to the RIXS spectra at some temperature T, Iₛ(T), can be obtained by Iₛ(T) = Fₛ(T)/(Fₚ(T) + Fₛ(T)). This measured s-like contribution Iₛ(T) at different temperatures is equal to a theoretically evaluated Iₛ(R, τ). The probability for a core hole decay at time t is exp(−t/τ). For a constant phonon scattering rate R, the probability that a single phonon scattering event has not yet happened until t is 1 − exp(−Rt). When we include multiphonon scattering with alternating sign [31], taking into account that an even number of AM \(\mid l\mid = 1\) transfers results in the same state (neglecting \(1 \geq 2\) because of vanishing DOS), we can evaluate the probability of observing the s-projected DOS in the spectrum through multiplying the decay and phonon scattering probabilities and integrating over time.
\[ I_s(R, \tau) = \int_0^\infty \frac{\exp (-t/\tau)}{\tau} \left( \sum_{n=0}^\infty (-1)^n \left[ 1 - \exp \left( -\frac{R}{n} \right) \right] \right) dt \]

\[ = \int_0^\infty \frac{\exp (-t/\tau)}{\tau [2 - \exp (-\frac{R}{\tau})]} dt. \]

We then link the measured s-like contributions found in the RIXS spectra at different temperatures with the calculated \( I_s(R, \tau) \) expression and apply the Si 2p core hole lifetime of \( \tau = 8 \) fs, \( I_s(T) = I_s(R, \tau = 8 \) fs). Thus we can determine, the AM transfer rate \( R \) at a particular temperature \( T \). Note that values for the Si 2p core hole lifetime as extracted from the natural lifetime broadening of the photoemission line range in the literature from 7 to 19 fs [37–43], with an average of about 13 fs.3 In order to be consistent with the data on crystalline silicon, we chose our reference lifetime to be 8 fs. The choice of the absolute value of the core hole lifetime remains arbitrary considering the range mentioned in literature (combined with the error bars in all those measurements).

3.2. CM transfer

In addition to the dipole selection rule, with RIXS for on resonance (and close to resonance) excitation there is also a CM (k) selection rule reflecting the conservation of CM in the process [35]: at the Si 2p resonance the core excited state is created with a specific CM through the excitation of an electron into a state in the conduction band with this CM. The core hole can only be filled with electrons having the same particular CM. The resulting part of the spectrum is called ‘coherent’.

The Si 2p RIXS at \( hv = 101.35 \) eV (on-resonance) excitation and for excitation energies detuned with –0.2 eV from resonance (RIXS at \( hv = 101.15 \) eV) were analyzed for different temperatures and compared with the RIXS for continuum excitation.

With RIXS for continuum excitation no specific crystal momenta are selected since the excited electron is ejected into vacuum. RIXS for continuum excitation can in this regard be treated as incoherent and the spectral shape directly represents the DOS as determined by the dipole selection rule (and possible AM transferring electron–phonon scattering events).

A resonantly measured spectrum always contains both contributions: an incoherent and a coherent part. This is a result of electron–phonon scattering in realistic systems. When scattering with a phonon occurs during the lifetime of the core hole, the energy of the electronic transitions is negligibly changed while the CM is completely randomized. This disturbs the coherence in the electronic transitions and the resulting spectral shape resembles again the dipole selected DOS, identical to what is measured with non-resonant excitation. From the relative weights of the incoherent and coherent parts of the spectra, it can thus be determined, if electron–phonon scattering occurred during the core hole lifetime. Quantitatively, the ratio of incoherent to coherent intensities in the RIXS on resonance is related to CM transfer times the effective RIXS duration time, e.g., the Si 2p core hole lifetime set at \( \tau = 8 \) fs in the case of the on-resonance excitation.3 By analyzing the incoherent and coherent part in Si 2p RIXS, we are

3 As said, in order to be consistent with the data on crystalline silicon, we chose our reference lifetime to be 8 fs. Nevertheless, for consideration of quantitative measurements one may choose to linearly scale the electron–phonon scattering parameters presented in this paper (for both silicon and silicon carbide) with 8/13 using the average of 13 fs that we obtained from the range from literature.
looking at the momentum transfer from phonons to electrons. While the RIXS process has its k-selectivity, this means that in order to obtain incoherent features in the RIXS, the phonons have to transfer momentum to the electrons.

To determine the relative weights of each part, the following procedure is applied: the RIXS on resonance and RIXS slightly detuned from resonance are compared with the RIXS for continuum excitation. All the RIXS spectra are normalized to their area. Subsequently, the RIXS at $h\nu = 101.35$ eV and measured with a small detuning in the incident energy from this resonance (RIXS at $h\nu = 101.15$ eV) are decomposed into a maximized fraction of the area-normalized RIXS for continuum excitation ($h\nu = 115.0$ eV) of the same temperature and a remaining coherent part. The fraction of the RIXS for continuum excitation accounts for the incoherent ($I_{\text{incoh}}$, non k-conserving) contribution to the RIXS measured at $h\nu = 101.35$ and $h\nu = 101.15$ eV excitation. Thus the ratio between the coherent ($I_{\text{coh}}$) and incoherent ($I_{\text{incoh}}$) emission is evaluated as a measure for the CM k randomization during the Si 2p core hole lifetime, which is here connected with electron–phonon scattering. Electron–electron scattering is ruled out in the excited state, since the thermal occupation of electrons in the conduction band above the band gap of about 3 eV is negligible and in the filled valence band there are no empty final states for electron–electron scattering available. Therefore the ratio between incoherent and coherent emission is connected to the electron–phonon coupling rate $R_{\text{ph}}$ by: $I_{\text{incoh}} / I_{\text{coh}} = \tau (\Omega) \times R_{\text{ph}}$, where $\tau (\Omega)$ is the effective RIXS duration time, e.g., the Si 2p core hole lifetime with the detuning energy $\Omega$ relative to the resonance energy, so $\Omega = 0$ for the resonance energy of 101.35 eV.

The lifetime of the core excited intermediate state $\tau$ changes when the incident energy is slightly detuned from resonance: $\tau (\Omega) = \hbar(\Omega^2 + I^2)^{-\frac{1}{2}} [34]$, where $\tau$ is expressed in its natural lifetime broadening $I$ (HWHM) and detuning energy $\Omega$.

In the case of silicon, detuning from resonance lead to a slightly different RIXS spectrum (see figure 2 in [31]). This is due to a peculiarity of the silicon band structure, where the conduction band minimum is not located at a high symmetry point in the band structure and thus has only a small density of states. Detuning from resonance lowers the resonant enhancement of the conduction band minimum and the RIXS from the highly symmetric X-point becomes dominating because of a higher DOS. In contrast, for 6H-SiC the conduction band minimum is located at the M and L points in k-space with a high DOS. Slight detuning does not strongly change the dominating contributions to the spectra and therefore the RIXS spectra for resonance excitation and for slightly detuned from resonance excitation should be quite similar.

However detuning from resonance changes the effective duration time of the scattering process, so that with detuning an additional measurement of the same process can be performed with a different reference timescale and the obtained results can be cross-checked.

### 3.3. Thermal evolution of angular/crystal momentum transfer

The thermal evolution of momentum transfer rates $R$ (either angular or CM) can be described by a constant contribution $A$ due to phonons created by core excited state lattice distortions and by a temperature-dependent part that is proportional to the phonon number. Since this method does not differentiate between contributing phonon modes but averages the scattering events over all contributing modes, the phonon number is modeled by a Bose–Einstein function for a single phonon mode with the averaged phonon energy of 78.6 meV (this value was obtained for 15R-
SiC, but the phonon spectra for the 6H and 15R polytypes do not differ much [44]). The thermal evolution of the momentum transfer rate ($Y$) may be written mathematically as

$$Y = A + \frac{1}{e^{\frac{E}{kT}} - 1} \times B,$$

where $\frac{1}{e^{\frac{E}{kT}} - 1}$ is the Bose–Einstein distribution for the average phonon number at a given temperature with the applied average phonon energy of 78.6 meV. $A$ and $B$ are fitting parameters for the temperature-independent and temperature-dependent electron–phonon scattering rates per average phonon respectively. Distinction between $A$ and $B$ for AM transfer and CM transfer is made with the proper subscripts.

In section 3.2 we mentioned that we can rule out the electron–electron scattering. However, the used x-ray probe leads to a high-energy excitation, which could lead to a larger possibility of electron–electron scattering. Since the energy of this x-ray probe is the same for all temperatures, the effect of the high-energy excitation on electron–electron scattering will only be part of the temperature-independent component $A_{CM}$ and $A_{AM}$.

4. Results

Figure 1 shows the measured Si 2p XAS (left plot) and the Si 2p RIXS (right plot) taken for three different incident photon energies. The XAS spectra display a broad maximum related to continuum excitation with an extra bump superimposed at energies below about 102 eV. This bump indicates a core-hole excitonic structure of finite width with a low-energy cut off at about 101.35 eV (for simplification this energy value at half the maximum resonance yield will be named on-resonance in the subsequent text). The Si 2p RIXS have been taken for primary
energies of 101.35 eV (on-resonance, curves B), 101.15 eV (−0.2 eV detuned from the resonance energy, curves A) and for continuum excitation at 115 eV (off-resonance, curves C). The Si 2p XAS is normalized to the maximum of the Si L$_3$-edge and all the Si 2p RIXS spectra are normalized to their area. The Si 2p XAS and RIXS spectra of 6H-SiC measured at room temperature (black lines) agree reasonably well with the 6H-SiC data published by Lüning et al [45], e.g. all the RIXS key features as presented in their paper are present and the Si 2p XAS at room temperature has a similar shape.

The Si 2p XAS spectra at different temperatures (left panel figure 1) show a slight shift of the Si L$_3$ absorption edge position to lower energy for increasing temperatures. For both the RIXS spectra at on-resonance excitation (figure 1, right panel, series B, $h\nu = 101.35$ eV, where this resonance energy is selected by taking the maximum of the derivative of the Si L$_3$-edge measured at room temperature) and at an excitation energy slightly detuned from resonance (figure 1, right panel, series A, $h\nu = 101.15$ eV) the feature at about 91 eV decreases with increasing temperature, while the intensity between 93 and 97 eV and even higher energies increases with increasing temperature. This behavior can as well be found in the Si 2p RIXS for continuum excitation (figure 1, right panel series C, $h\nu = 115.0$ eV): the band around 91 eV decreases with increasing temperature and the band around 97 eV increases with temperature but only slightly as compared to the on-resonance and the slightly detuned RIXS spectra. In all the RIXS spectra there is a small shift of the band between 97–100 eV to higher energy with increasing temperature. These small energetic changes in combination with the shift of the Si L$_3$ absorption edge point to a decrease in the band gap energy with temperature. A detailed discussion is beyond the scope of this paper and will be conducted elsewhere [46]. The changes in the features of the RIXS spectra with temperature will be dealt with in the following subsections.

4.1. AM transfer

First we focus on the RIXS for continuum excitation spectra measured at different temperatures (right panel figure 1, series C). For these spectra, there should be a strong correspondence to the shape of silicon s-projected DOS. The top panel of figure 2 shows the ground state valence silicon s- and p-projected DOS of 6H-SiC (without core holes) as calculated by Gavrilenko et al [47] and the middle panel of figure 2 presents the differences in the RIXS for continuum excitation ($h\nu = 115.0$ eV) at different temperatures compared to the RIXS for continuum excitation at room temperature (25 °C). We focus on the RIXS for continuum excitation, because no overlaid resonant effects, no coupling of the valence-band electrons to the excited electron and only minor shake-up effects are expected and thus a comparison with the calculated DOS is more straightforward. For a better comparison with the experimental RIXS differences, the silicon s-projected DOS in the top panel is multiplied by −1. Comparing the two top panels in figure 2 it is evident that the differences in the RIXS at different temperatures are closely connected to the shapes of s- and p-projected DOS.

As already mentioned in the theoretical section, the dipole selection rule applies to Si 2p RIXS. Hence in the RIXS only transitions from s- and d-states to the Si 2p are allowed. Nonetheless, from the connection between the two top panels in figure 2, the p-projected DOS contribution to the RIXS for continuum excitation increases with temperature (as compared to room temperature), while the relative s-projected DOS contribution to the spectra decreases.
For quantitative analysis of the AM transfer, the RIXS spectra for continuum excitation were decomposed in s- and p-state contributions using the calculations of the silicon s- and p-projected DOS from the top panel of Figure 2. For selected regions marked with I, II and III in the two top panels of Figure 2 the integrated areas of the calculated silicon s-projected DOS (DOSs), p-projected DOS (DOSp) and the integrated areas for the RIXS for continuum excitation (IRIXS) at different temperatures were obtained. For this analysis we used the full RIXS spectra from Figure 1 instead of the difference spectra shown in the middle panel of Figure 2. The latter only illustrates the strong connection between the projected DOS and the changes in the RIXS with temperature.

The three analyzed regions were selected based on the relative amount of s- and p-projected DOS: area I and III contain mainly s- or p-projected DOS respectively, while area II contains both. Furthermore, there are dissimilarities between the experimental RIXS differences for continuum excitation and the calculated DOS. The areas have been chosen to avoid differing regions.

The main discrepancy between the calculated s- and p-projected DOS and the measured RIXS differences is that the calculated DOS drops to zero at lower energies than the RIXS data close to the band gap. Density functional theory in the local-density approximation as used by

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**Figure 2.** Experimental determination of angular momentum transfer. Top panel: Silicon s- and p-projected DOS of 6H-SiC as calculated by Gavrilenko et al [47] and energy aligned as stated in the main text. The s-projected DOS is multiplied by \(-1\). Middle panel: difference between the RIXS for continuum excitation at \(T = 300^\circ C\) (red), 600°C (green) or 900°C (blue) and the RIXS for continuum excitation at 25°C. Bottom panel: angular momentum (AM) transfer rates in fs\(^{-1}\) versus temperature (K). The dotted line is a fit using the thermal evolution of the angular momentum transfer rate with the average phonon energy of 78.6 meV and the adjustable parameters \(A_{AM} = 0.015\) (fs\(^{-1}\)) and \(B_{AM} = 0.10\) (fs\(^{-1}\)). The estimated standard deviations of \(A_{AM}\) and \(B_{AM}\) are respectively \(\sigma_{A} = 0.025\) fs\(^{-1}\) and \(\sigma_{B} = 0.03\) fs\(^{-1}\).
Gavrilenko et al [47] shows in general deviations from experimental data near the band gap. Valence-band states in semiconductors contributing to the electronic ground state density tend to agree with experimental shapes, although the total valence-band width may be smaller [48–50], which is similarly observed here comparing the calculated DOS with the RIXS differences for 6H-SiC. Note that more recent DOS calculations on 6H-SiC (for example [51, 52]) find similar s-DOS and p-DOS as obtained from the calculations by Gavrilenko et al [47]. Another factor that contributes to the difference in valence-band width between the RIXS for continuum excitation and the calculated DOS is the temperature. The calculations were performed at 0 K, while the RIXS was measured at higher temperatures and the results on the RIXS presented above show that the VBM is moving to higher energy with increasing temperature. Overall, the exact reproduction of the size of the band gap as well as the valence band maximum with \textit{ab initio} methods is challenging and can only be solved by adding the effects of electrons in excited states and valence holes in the optical spectrum [20] and by including improved exchange and correlation in the calculation methods.

We would like to point out that the feature appearing in the middle panel around 99 eV increasing for the 300–900 °C is an indirect result of the shift of the valence band maximum with temperature shortly mentioned above. In a separate paper we analyze the band gap, the valence band maximum and conduction band minimum of 6H-SiC as a function of temperature [46]. The RIXS spectra indicated with C in the left panel of figure 1 do not seem to show this valence band maximum shift, but after zooming in one may recognize a small but non-negligible shift in the valence band maximum as a function of temperature [46]. Nevertheless, we want to make the point that we are allowed to make a comparison between calculated DOS and RIXS. Since the RIXS studies mostly the final state (valence excited states) and with the energy losses relatively close to the elastic line in the present RIXS spectra, the RIXS process boils down to mostly single particle excitations which can be rather well described with DFT. As said, DFT is only an approximation, but we only use it to extract the s- and p-projected DOS. Although, the energies in DFT are slightly wrong, the symmetry of the underlying states is rather well reproduced by DFT. Thus in essence, the information that we extract from DFT is rather coarse and does not rely on details of the approximations in the calculations.

The bottom panel of figure 2 presents the estimates of the AM transfer from the analysis of the selected areas in the RIXS for continuum excitation areas at different temperatures with the calculated s- and p-projected DOS of 6H-SiC in the same selected ranges. For the measurements at \( T=1173 \) K, the standard deviation is much larger than at the other temperatures. This is due to a large background in the measured data as an artifact produced by our heating device which is only significant at this elevated temperature. The AM transfer rates \((Y)\) are fitted using \( A_{AM}=0.015(25) \text{ } \text{fs}^{-1} \) and \( B_{AM}=0.10(3) \text{ } \text{fs}^{-1} \).

For silicon the \( A_{AM}=0.044 \text{ } \text{fs}^{-1} \) and the \( B_{AM}=0.0035 \text{ } \text{fs}^{-1} \) [31] are quite different from the values obtained for 6H-SiC. While the temperature-independent contribution is lower for 6H-SiC, the temperature-dependent electron–phonon scattering rate per average phonon is roughly thirty times higher for 6H-SiC. Since the standard deviation in the temperature-independent electron–phonon scattering for AM transfer is larger than the estimated value of \( A_{AM} \), we refrain from a detailed comparison between silicon and 6H-SiC in this regard. However, we will come back to the temperature-dependent \( B_{AM} \) in the discussion section below.
4.2. CM transfer

For RIXS on-resonance and excited close to the resonance, there is CM (k) selectivity [35] on top of the dipole-selection rule. In the present study the Si 2p RIXS at $h\nu = 101.35$ eV (on-resonance) excitation and for excitation energies detuned with $\Delta \nu = 0.2$ eV from resonance (RIXS at $h\nu = 101.15$ eV) are analyzed for different temperatures and compared with the RIXS for continuum excitation, where no specific crystal momenta are selected.

The top panel in figure 3 presents the spectra of RIXS at resonance, $h\nu = 101.35$ eV, excitation (black solid) and for continuum excitation ($h\nu = 115.0$ eV, red, dotted) at room temperature. Qualitative comparison between the two spectra shows that the k-conserving term is almost solely present in the band at 90–92 eV. The on-resonance Si 2p excitation of 6H-SiC leads to core hole excited states at well-defined L and M points in k space [53]. The band dispersion relation of 6H-SiC [54] with a band containing bound L and M states at about $\Delta = 8$ eV from the VBM (and approximately $\Delta = 11$ eV from the CBM) supports the assignment of the k-conserving term to this band at 90–92 eV. In addition, we detect a significant contribution without k-selectivity in the RIXS at $h\nu = 101.35$ eV excitation. The high-energy side of the RIXS for continuum excitation extends to higher energy than the RIXS at resonant excitation, which is due to the so-called spectator shift in RIXS at resonance excitation that screens the core hole and leads to a downshift in the XES energies for RIXS at resonance excitation compared to RIXS for continuum excitation [55].

All the obtained $R_{ph}$ results following the analysis procedure mentioned in the section 3.2 are presented in the bottom panel of figure 3 (black squares for on-resonance data, red dots for...
the \(-0.2\) eV detuned data and green triangles for the average of both data) with their respective standard deviation. The standard deviation is not constant and is higher at some temperatures due to shorter acquisition times. In addition the standard deviation at the highest temperature is influenced by a large background in the RIXS measurements due to an artifact produced by our heating device as mentioned before in the analysis of AM transfer.

The line in the bottom panel of figure 3 accounts for the thermal evolution of the CM transfer with the fitted parameters \(A_{\text{CM}} = 0.8(4)\) fs\(^{-1}\) and \(B_{\text{CM}} = 1.8(8)\) fs\(^{-1}\). The values for \(A_{\text{CM}}\) and \(B_{\text{CM}}\) obtained for 6H-SiC are substantially higher than the values obtained for silicon. The \(A_{\text{CM}}\) for crystalline silicon was \(\sim 0.4\) fs\(^{-1}\) [31] and for 6H-SiC the obtained \(A_{\text{CM}}\) is twice as high. For crystalline silicon, the value of the temperature-dependent electron–phonon scattering rate per thermally excited average phonon based on CM transfer \(B_{\text{CM}}\) was 0.2 fs\(^{-1}\) [31]. For 6H-SiC, the obtained value of \(B_{\text{CM}}\) is nine times higher. Comparing the ratio between angular and CM transfer per phonon the ratio is \(B_{\text{AM}}/B_{\text{CM}} = 0.06\). This means that about 6% of the thermally excited phonons carry a nonzero AM, which is in the same order of magnitude as the value of 2% obtained for silicon before [31], but still this ratio is approximately three times as high for 6H-SiC as compared to silicon.

5. Discussion

Here we focus on discussing the differences between silicon and 6H-SiC in the angular and CM transfer and the respective electron–phonon scattering rates. In table 1 some parameters that affect the electronic and phonon DOS are shown for silicon and 6H-SiC. It is not unexpected that the electron–phonon scattering rates of silicon and 6H-SiC are different, since there are numerous differences between the two semiconductors, however that the electron–phonon scattering rates of 6H-SiC are higher than the ones of silicon cannot be easily interpreted from these parameters.

| Parameter                                      | 6H-SiC          | Silicon         |
|------------------------------------------------|-----------------|-----------------|
| Band gap (indirect) energy (eV)                | 3.1\(^{\text{b}}\) | 1.12\(^{\text{c}}\) |
| Angular momentum transfer—temperature-independent contribution \(A_{\text{AM}}\) (fs\(^{-1}\)) | 0.015 (0.025)\(^{\text{a}}\) | 0.044 [31] |
| Angular momentum transfer—temperature-dependent contribution \(B_{\text{AM}}\) (fs\(^{-1}\)) | 0.1 (0.03)\(^{\text{a}}\) | 0.0035 (0.0004) [31] |
| Crystal momentum transfer—temperature-independent contribution \(A_{\text{CM}}\) (fs\(^{-1}\)) | 0.8 (0.4)\(^{\text{a}}\) | 0.4 [31] |
| Crystal momentum transfer—temperature-dependent contribution \(B_{\text{CM}}\) (fs\(^{-1}\)) | 1.8 (0.8)\(^{\text{a}}\) | 0.20 (0.02) [31] |
| Angular/crystal momentum transfer (%)          | 6\(^{\text{a}}\) | 2 [31] |
| Average phonon energy (meV)                    | 78.6\(^{\text{[58]}}\) | 38\(^{\text{[58]}}\) |
| Si 2p excitation to K-point                    | M/L\(^{\text{b}}\) | (close to) X\(^{\text{c}}\) |
| Phonon branches expected (#)                   | 36 [19, 59] | 24 [19, 59] |
Due to the highly symmetric unit cell, crystalline silicon shows fewer bands in the band structure [56] compared to 6H-SiC [54]. The lower amount of bands could suppress the electron–phonon scattering in silicon, since the phase space of final states in electron–phonon scattering is smaller compared to 6H-SiC. An additional cause for the electron–phonon scattering differences is the relative mass of the atoms. Carbon is a much lighter element than silicon, thus carbon atoms may more easily move and as a consequence Si–C bonds may vibrate more strongly than silicon–silicon bonds. The average mass of an atom in SiC is 20.05 (with silicon and carbon atoms in a 1:1 ratio) and 28.09 in silicon, which is a factor 1.4 different. Due to the lighter surrounding carbon atoms, also the (vibrational) adaptation to changes, such as to the creation of a core hole, can be faster. Therefore faster and more extreme relaxation processes in presence of the core hole will occur for a Si 2p core hole in SiC than in silicon. Due to the local movements of the carbon atoms surrounding the silicon with a core hole, core hole initiated phonons could evolve, which we can quantify in the temperature-independent momentum transfer, the values of $A_{AM}$ and $A_{CM}$. We indeed observe an increase in the $A_{CM}$ for SiC compared to silicon, but we do not see the same effect in $A_{AM}$. All the above mentioned gives only slight indications for the difference in the electron–phonon scattering rates between 6H-SiC and silicon and does not necessarily show why the electron–phonon scattering rates of 6H-SiC are higher than silicon. Monserrat and Needs have calculated electron–phonon coupling strengths for diamond, silicon and cubic silicon carbide [57] and discuss as well the difference in the electron–phonon coupling strengths. Although they recognize the fact that the lighter carbon atoms may contribute to the electron–phonon coupling strength, they conclude that this is not enough to explain the difference in strength between diamond, silicon and cubic silicon carbide.

In contrast to silicon, SiC has valence- and conduction-band electron density more strongly localized on the silicon atoms. In calculations on the valence-band DOS, Johansson et al found a small contribution of d-projected DOS at the silicon sites in 6H-SiC [52] while d-projected valence-band DOS is often assumed to be negligible in crystalline silicon. Hopfield pointed out that the electron–phonon coupling constant depends strongly on the density of localized (d-) electrons [60]. In general valence d-electrons are more localized to atoms than valence s- and p-electrons.

The driving force of electron–phonon scattering is how the electronic system reacts to nuclear motions and electrons that are more strongly localized to the nucleus show a bigger effect than more delocalized states and it is well known from studies on superconductors that relatively free valence electrons screen the electron–phonon coupling [19, 60]. In the present study we have shown that in 6H-SiC electron–phonon coupling is larger. This is due to a larger contribution of localized d-symmetric states at the silicon atoms. From the DOS calculation of Johansson et al for 6H-SiC [52] the relative s-, p- and d-projected DOS weights at the silicon atoms in the upper 8 eV of the valence-band are 38.6, 50.6 and 10.8% respectively. In silicon, the corresponding numbers are 9.0, 86.6 and 4.4%. Thus in crystalline silicon, electron–phonon coupling is effectively screened by the free valence electrons and the observed rates are therefore smaller than for 6H-SiC.

Note that we have neglected the d-projected DOS in our analysis so far. While the d-projected DOS does not play a specific role in the analysis of the CM transfer it enters the AM transfer rate analysis. We can anyway safely neglect it due to the small contribution to the overall shape of the spectra, which is close to the limit of our resolution. Besides, the effects were neglected for both silicon and 6H-SiC. Even when the d-projected DOS would have been
taken into account we suspect that the $B_{AM}$ of 6H-SiC would remain more than 20 times as large as the $B_{AM}$ of silicon, because the relative weight of the d-projected DOS remains relatively small in comparison to the s- and p-projected DOS for both materials. Although the contribution to the spectral shapes and thus to our analysis is small, it can still strongly influence the general size of electron–phonon scattering rates.

Considering that SiC light emitters have developed, while SiC has an indirect band gap, we notice that the AM transfer rate in SiC (0.1 fs$^{-1}$) is on the order of the CM transfer rate in silicon (0.2 fs$^{-1}$), while the CM transfer rate due to electron–phonon scattering in 6H-SiC is much higher (1.8 fs$^{-1}$) than in silicon and this huge difference makes SiC a potentially better light emitter than expected due to its indirect band gap.

As another final discussion point, we would like to mention that electron–phonon coupling has been studied before with RIXS (for example [61–64]), focusing on the copper L- and K-edge and the progression of some phonon modes. In those particular cases they could measure phonons directly with their RIXS resolution, but unfortunately for the present silicon 2p RIXS measurements we cannot achieve such high resolution and within our resolution of 0.2 eV we are not able to distinguish the different phonon modes (e.g., $A_1$, $B_1$, E etc) overlapping in energy due to the relative low symmetry directly next to the elastic scattering line. The phonon dispersion of 6H-SiC [65] is rather complicated: there is much overlap of the different phonon modes in k-space. Even with the best resolution known for RIXS in this energy interval it is difficult or even impossible to observe anything else than just a broad feature. Nevertheless, this means that for systems that have a complicated band structure and phonon structure, the method as applied in the present paper has clear advantages.

6. Summary and conclusions

The interplay between electron localization and the angular and CM transfer in electron–phonon scattering was studied applying RIXS at the silicon 2p edges of 6H-SiC in comparison to crystalline silicon. Experimentally we employed the scattering duration time of RIXS at the Si 2p core levels in combination with the symmetry selection rules of RIXS as an ultrafast probe for electron–phonon scattering. Additionally, the sample temperature allowed varying the number of phonons in the system. Electron–phonon scattering rates in 6H-SiC were determined to be 1.8 fs$^{-1}$ per average phonon for CM transfer in comparison to 0.2 fs$^{-1}$ in crystalline silicon. The estimated electron–phonon AM transfer rate per average phonon in 6H-SiC was 0.1 fs$^{-1}$ and this was much higher compared to 0.0035 fs$^{-1}$ for crystalline silicon. Besides these temperature-dependent values, temperature-independent electron–phonon scattering rates for crystal and AM transfer were determined as well. The discussion provided that the higher electron–phonon scattering rates in 6H-SiC are dominated by the stronger electron localization at the silicon atoms in 6H-SiC in comparison to crystalline silicon. Smaller contributions arise from the lighter carbon versus silicon atomic masses and to the difference in the structures or the local symmetry.

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References

[1] Dagotto E 2005 Complexity in strongly correlated electronic systems Science 309 257–62
[2] Bardeen J, Cooper L N and Schrieffer J R 1957 Theory of superconductivity Phys. Rev. 108 1175–204
[3] Driza N et al 2012 Long-range transfer of electron–phonon coupling in oxide superlattices Nat. Mater. 11 675–81
[4] Reznik D, Pintschovius L, Ito M, Likubo S, Sato M, Goka H, Fujita M, Yamada K, Gu G D and Tranquada J M 2006 Electron–phonon coupling reflecting dynamic charge inhomogeneity in copper oxide superconductors Nature 440 1170–3
[5] Liu Z K et al 2013 Measurement of coherent polarons in the strongly coupled antiferromagnetically ordered iron-chalcogenide Fe1.02Te using angle-resolved photoemission spectroscopy Phys. Rev. Lett. 110 037003
[6] Gadermaier C, Alexandrov A S, Kabanov V V, Kusar P, Mertelj T, Yao X, Manzioni C, Brida D, Cerullo G and Mihailovic D 2010 Electron–phonon coupling reflecting dynamic charge inhomogeneity in copper oxide superconductors Nature 440 1170–3
[7] Norman M R 2011 The challenge of unconventional superconductivity Science 332 196–200
[8] Wang F and Lee D-H 2011 The electron-pairing mechanism of iron-based superconductors Science 332 200–4
[9] Weber F, Rosenkranz S, Castellan J P, Osborn R, Karapetrov G, Hott R, Heid R, Bohnen K P and Alatas A 2011 Electron–phonon coupling and the soft phonon mode in TiSe2 Phys. Rev. Lett. 107 266401
[10] Zhu X, Santos L, Howard C, Sankar R, Chou F C, Chamon C and El-Batanouny M 2012 Electron–phonon coupling on the surface of the topological insulator Bi2Se3 determined from surface-phonon dispersion measurements Phys. Rev. Lett. 108 185501
[11] Pan Z H, Fedorov A V, Gardner D, Lee Y S, Chu S and Valla T 2012 Measurement of an exceptionally weak electron–phonon coupling on the surface of the topological insulator Bi2Se3 using angle-resolved photoemission spectroscopy Phys. Rev. Lett. 108 187001
[12] Attaccalite C, Wirtz L, Lazzeri M, Mauri F and Rubio A 2010 Doped graphene as tunable electron–phonon coupling material Nano Lett. 10 1172–6
[13] Zhu J, Badalyan S M and Peeters F M 2012 Electron–phonon bound states in graphene in a perpendicular magnetic field Phys. Rev. Lett. 109 185501
[14] Hoesch M, Piekarz P, Bosak A, Le Tacon M, Krisch M, Kozlowski A, Oles A M and Parlinski K 2013 Anharmonicity due to electron–phonon coupling in magnetite Phys. Rev. Lett. 110 207204
[15] de Jong S et al 2013 Speed limit of the insulator–metal transition in magnetite Nat. Mater. 12 882
[16] Koopmans B, Malinowski G, Dalla Longa F, Staiauf D, Fähnle M, Roth T, Cinchetti M and Aeschlimann M 2010 Explaining the paradoxical diversity of ultrafast laser-induced demagnetization Nat. Mater. 9 259
[17] Kimel A V, Kimilyuk A, Tsvetkos A, Pisarev R V and Rasing T 2004 Laser-induced ultrafast spin reorientation in the antiferromagnet TmFeO3 Nature 429 850–3
[18] Radu I et al 2011 Transient ferromagnetic-like state mediating ultrafast reversal of antiferromagnetically coupled spins Nature 472 205–8
[19] Ziman J M 1960 Electrons and Phonons—The Theory of Transport Phenomena in Solids (New York: Oxford University Press)
[20] Baroni S, De Gironcoli S, Dal Corso A and Giannozzi P 2001 Phonons and related crystal properties from density-functional perturbation theory Rev. Mod. Phys. 73 515–62
[21] Koga K and Yamaguchi T 1991 Single-crystals of SiC and their application to blue LEDs Prog. Cryst. Growth Charact. Mater. 23 127–51
[22] Edmond J, Kong H, Suvorov A, Waltz D and Carter C 1997 6H-Silicon carbide light emitting diodes and UV photodiodes Phys. Status Solidi A 162 481–91
[23] Syväjärvi M et al 2012 Fluorescent SiC as a new material for white LEDs Phys. Scr. 81 014002
[24] Dakshinamurthy S, Quick N R and Kar A 2007 Temperature-dependent optical properties of silicon carbide for wireless temperature sensors J. Phys. D: Appl. Phys. 40 353–60
[25] Nava F, Bertuccio G, Cavallini A and Vittone E 2008 Silicon carbide and its use as a radiation detector material *Meas. Sci. Technol.* **19** 102001

[26] Ruddy F H, Dulloo A R, Seidel J G, Das M K, Sei-Hyung R and Agarwal A K 2006 The fast neutron response of 4H silicon carbide semiconductor radiation detectors *IEEE Trans. Nucl. Sci.* **53** 1666–70

[27] Castelletto S, Johnson B C, Ivady V, Stavrias N, Umeda T, Gali A and Ohshima T 2014 A silicon carbide room-temperature single-photon source *Nat. Mater.* **13** 151–6

[28] Boretti A 2014 Optical materials: silicon carbide’s quantum aspects *Nat. Photon.* **8** 88–90

[29] Bernstein N, Gotsis H J, Papconstantopoulos D A and Mehl M J 2005 Tight-binding calculations of the band structure and total energies of the various polytypes of silicon carbide *Phys. Rev. B* **71** 075203

[30] Beyer M and Föhlisch A 2011 A soft x-ray approach to electron–phonon interactions beyond the Born–Oppenheimer approximation *J. Electron Spectrosc. Relat. Phenom.* **184** 313–7

[31] Beyer M, Hennies F, Deppe M, Suljoti E, Nagasono M, Wurth W and Föhlisch A 2009 Dynamics of electron–phonon scattering: crystal- and angular-momentum transfer probed by resonant inelastic x-ray scattering *Phys. Rev. Lett.* **103** 237401

[32] Kunnus K et al 2012 A setup for resonant inelastic soft x-ray scattering on liquids at free electron laser light sources *Rev. Sci. Instrum.* **83** 123109

[33] Föhlisch A, Feulner P, Hennies F, Fink A, Menzel D, Sanhez-Portal D, Echenique P M and Wurth W 2005 Direct observation of electron dynamics in the attosecond domain *Phys. Rev. Lett.* **95** 173001

[34] Gel'mukhanov F and Agren H 1999 Resonant x-ray Raman scattering *Phys. Rep.* **312** 87–330

[35] Kotani A and Shin S 2001 Resonant inelastic x-ray scattering spectra for electrons in solids *Rev. Mod. Phys.* **73** 203–46

[36] Jimenez-Mier J, Ederer D L, Schuler T and Callcott T A 2003 Direct evidence for 3p → 2p non-dipole x-ray emission in transition metals *J. Phys. B: At. Mol. Opt. Phys.* **36** L173–80

[37] Tong X, Ohuchi S, Tanikawa T, Harasawa A, Okuda T, Aoyagi Y, Kinoshita T and Hasegawa S 2002 Core-level photoemission of the Si(111)-21 × 21-Ag surface using synchrotron radiation *Appl. Surf. Sci.* **190** 121–8

[38] Uhrberg R I G, Kaurila T and Chao Y C 1998 Low-temperature photoemission study of the surface electronic structure of Si(111)-7 × 7 *Phys. Rev. B* **58** R1730–3

[39] Ley L, Reichardt J and Johnson R L 1982 Static charge fluctuations in amorphous silicon *Phys. Rev. Lett.* **49** 1664–7

[40] Bringans R D, Olmstead M A, Uhrberg R I G and Bachrach R Z 1987 Core level spectroscopy of the GaAs-on-Si interface *J. Vac. Sci. Technol. A* **5** 2141–2

[41] An K S, Hwang C C, Kim Y K, Cho E S, Park C Y, Pukird S, Kakizaki A, Okuda T and Kinoshita T 2002 Atomic and electronic structures of Si(111)1 × 1-Sb surface: core-level shifts and surface states *Surf. Sci.* **513** 49–56

[42] Hricovini K et al 1993 Electronic structure and its dependence on local order for H/Si(111)-(1×1) surfaces *Phys. Rev. Lett.* **70** 1992–5

[43] Zschornack G 2007 *Handbook of X-Ray Data* (Berlin: Springer)

[44] Patrick L, Choyke W J and Hamilton D R 1963 Optical properties of 15R SiC—luminescence of nitrogen-exciton complexes, and interband absorption *Phys. Rev. B* **59** 10573–82

[45] Lüning J, Eisebitt S, Rubensson J E, Ellmers C and Eberhardt W 1999 Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy *Phys. Rev. B* **59** 10573–82

[46] Miedema P S, Beyer M, Könecke R, Schiwietz G and Föhlisch A 2014 Thermal evolution of the band edges of 6H-SiC: x-ray methods compared to the optical band gap *J. Electron Spectrosc. Relat. Phenom.* **197** 37–42

[47] Gavrilin V I, Postnikov A V, Klyui N I and Litovchenko V G 1990 Energy-band structure and optical-properties of Wurtzite-structure silicon-carbide crystals *Phys. Status Solidi B* **162** 477–87

[48] Johnson K A and Ashcroft N W 1998 Corrections to density-functional theory band gaps *Phys. Rev. B* **58** 15548–56
[49] Seidl A, Görling A, Vogl P, Majewski J A and Levy M 1996 Generalized Kohn–Sham schemes and the band-gap problem Phys. Rev. B 53 3764
[50] Persson C, Nur O, Willander M, de Andrade e Silva E A and da Silva A F 2006 Electronic band-edge structure, effective masses, and optical absorption of Si_{1-x}Ge_x using an extended FPLAPW/VCA/LDA + U computational method Braz. J. Phys. 36 447–50
[51] Persson C and Lindefelt U 1997 Relativistic band structure calculation of cubic and hexagonal SiC polytypes J. Appl. Phys. 82 5496–508
[52] Johansson L I, Owman F, Martensson P, Persson C and Lindefelt U 1996 Electronic structure of 6H-SiC J. Appl. Phys. 82 5496–508
[53] Siklitsky V and Tolmatchev A 2013 Electronic archive new semiconductor materials. Characteristics and properties www.ioffe.ru/SVA/NSM/introduction.html visited April
[54] Cheng W, Ying M-J, Zhang F-S, Zhou H-Y and Ren S-F 2011 Density functional study on helium and hydrogen interstitials in silicon carbide Nucl. Instrum. Methods Phys. Res. B 269 2067–74
[55] Skytt P, Glans P, Gunnelin K, Guo J, Nordgren J, Luo Y and Agren H 1997 Role of screening and angular distributions in resonant x-ray emission of CO Phys. Rev. A 55 134–45
[56] Noffsinger J, Kioupakis E, Van de Walle C G, Louie S G and Cohen M L 2012 Phonon-assisted optical absorption in silicon from first principles Phys. Rev. Lett. 108 167402
[57] Monserrat B and Needs R J 2014 Comparing electron–phonon coupling strength in diamond, silicon, and silicon carbide: first-principles study Phys. Rev. B 89 214304
[58] Pässler R 2003 Semi-empirical descriptions of temperature dependences of band gaps in semiconductors Phys. Status Solidi B 236 710–28
[59] Kittel C 2005 Introduction to Solid State Physics (Hoboken, NJ: Wiley)
[60] Hopfield J J 1969 Angular momentum and transition-metal superconductivity Phys. Rev. 186 443–51
[61] Ament L J P, Van Veenendaal M and Van Den Brink J 2011 Determining the electron–phonon coupling strength from resonant inelastic x-ray scattering at transition metal L-edges Europhys. Lett. 95 27008
[62] Hancock J N, Chabot-Couture G and Greven M 2010 Lattice coupling and Franck–Condon effects in K-edge resonant inelastic x-ray scattering New J. Phys. 12 033001
[63] Abbamonte P, Burns C A, Isaacs E D, Platzman P M, Miller L L, Cheong S W and Klein M V 1999 Resonant inelastic x-ray scattering from valence excitations in insulating copper oxides Phys. Rev. Lett. 83 860–3
[64] Lee W S et al 2013 Role of lattice coupling in establishing electronic and magnetic properties in quasi-one-dimensional cuprates Phys. Rev. Lett. 110 265502
[65] Dorner B, Schober H, Wonhas A, Schmitt M and Strauch D 1998 The phonon dispersion in 6H-SiC investigated by inelastic neutron scattering Eur. Phys. J. B 5 839–46