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Temperature-induced evolutions in critical point optical transitions in HfS₂ investigated by spectroscopic ellipsometry



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ABSTRACT

A thorough understanding of the temperature-dependent optical properties and underlying physical mechanisms of a novel material is critical for the optimization of related optoelectronic devices. In this study, we comprehensively investigate the optical properties of the transition metal dichalcogenide HfS_2 over a broadband energy range of 0.75–5.91 eV with the temperatures changing from 100 K to 600 K by using the spectroscopic ellipsometry, critical point analysis, and first-principles calculations. The temperature-dependent dielectric functions are determined, and seven critical points (A–G) and their associated optical transitions are quantitatively revealed. We found that the central energies of these critical points exhibit temperature-induced blueshifts, consistent with the Varshni equation and Bose-Einstein model. The behavior of the critical points is significantly different as affected by thermal expansion and electron-phonon interactions of varying degrees. Due to the temperature-induced reversible phase transition of HfS_2 , critical points C and E exhibit dramatically increasing broadening and ultimately disappear. The locations of these optical transitions in the Brillouin zone and the involved carriers are further identified through energy band structure and projected density of states by combining the critical points analysis and first-principles calculations.

1. Introduction

Transition-metal dichalcogenides (TMDCs) have been regarded as one of the most promising materials for innovative nano-electronic and optoelectronic devices, attracting significant attentions over the past decade [1–6]. Their unique van der Waals layered structures [7] contribute to exceptional optical, electrical and thermal properties, such as tunable band gap [8–10], high carrier mobility [11], photoluminescence [12], induced optical anisotropy [13] and high thermal conductivity [14]. Numerous novel devices based on TMDCs have been researched and developed, including photodetectors [15], field-effect transistors [16], phototransistors [17], sensors [18], and solar cells [19].

The chemical formula of TMDCs is MX₂, where M represents a transition metal element from group IVB, VB, or VIB, and X denotes a group VIA element, typically sulfur (S), selenium (Se), or tellurium (Te). Hafnium disulfide (HfS₂), a member of the group IVB TMDCs, is predicted to demonstrate higher carrier mobility and greater tunneling

current density compared to the highly regarded group VIB TMDCs, such as MoS_2 and WS_2 [20]. The calculated acoustic-photon-limited mobility of HfS_2 at room temperature is up to $\sim 1800 \text{ cm}^2 V^{-1} s^{-1}$ compared to 340 cm² $V^{-1} s^{-1}$ for MoS_2 [21], making HfS_2 suitable for transistors [22], photodetectors [23,24] and photocatalysts [25]. However, the heat is inevitably generated during device operations. In order to better guide and optimize the design of HfS_2 -based optoelectronic devices, it is crucial to accurately characterize the optical properties of HfS_2 and reveal the temperature dependencies in them.

In recent years, several methods have been utilized to study the optical properties of HfS_2 and the effect of temperature. Zhao et al. calculated the energy band structures and dielectric functions of bulk and monolayer HfS_2 using first principles, and found that the bandgap calculated by the HSE06 hybrid functional method is the closest to experiment [26]. Kowalski et al. extracted the dielectric function of HfS_2 in the mid- and far-infrared bands by transmission and reflection spectroscopy, and found that it has a very broad Reststrahlen band, which

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greatly exceeds that of the Mo-based and W-based TMDCs due to the more than seven-fold increase in the Born effective charge of HfS_2 [27]. Lin et al. determined the temperature-dependent band gap of HfS_2 using absorption spectroscopy, revealing that its band gap has a negative temperature coefficient [28]. Antoniazzi et al. systematically studied the Raman spectra of bulk HfS_2 at temperatures of 5–350 K and found a blueshift in the A_{1g} mode as well as a blueshift in the E_g mode at low temperatures but a transition to a redshift at high temperatures [29]. Najmaei et al. researched and elucidated the anomalous high temperature coefficients of the carriers of HfS_2 [30]. These studies demonstrate the excellent optical properties of HfS_2 and its sensitivity to temperature. However, experimental measurements of the dielectric function of HfS_2 are still lacking in the UV–visible–NIR range, and no research has been reported focusing on its temperature-dependent optical behavior.

The temperature dependence of optical properties in crystalline materials is mainly governed by two physical mechanisms: lattice thermal expansion and electron-phonon interactions [31]. These factors can significantly influence the electronic band structure [32] and lead to shifts in interband transition energies, thereby modifying the dielectric response [33]. То comprehensively understand these temperature-induced effects in HfS₂, both experimental and theoretical approaches are essential. First-principles calculations provide an effective means to isolate and evaluate the impact of each mechanism. Specifically, the lattice thermal expansion can be estimated using the calculated thermal expansion coefficients [34], while the electron-phonon interaction can be described using the Allen-Heine-Cardona (AHC) theory [35-38]. Together, these approaches enable a detailed analysis of the temperature-dependent optical response.

In this work, we present a comprehensive study on the temperature dependence of the optical properties of HfS2. Raman spectra are used to determine the temperature-dependent phonon behaviors. The spectroscopic ellipsometry (SE) is utilized to accurately and quantitatively determine the dielectric functions and complex refractive indices of HfS_2 at different temperatures of 100-600 K over a broadband energy range of 0.75–5.91 eV. By combining the critical point (CP) analysis and firstprinciples calculations, seven different CPs marked as A-G are identified from the dielectric functions, and detailed information of these corresponding CP optical transitions are quantitatively revealed. When the temperature increases from 100 K to 600 K, the center energies of CPs A-G are blue-shifted, originating from the increase of the optical band gap due to the faster decrease of the exciton binding energy than the decrease of the band gap. And the blueshift of CPs aligns with the Varshni equation and the Bose-Einstein model. Due to lattice thermal expansion and electron-phonon interactions, the amplitudes and broadening factors of CPs A-G vary with temperature, with CP D and G having the weakest and strongest electron-phonon interactions, respectively. However, CPs C and E disappear at high temperatures as a result of a temperature-induced reversible phase transition. In addition, the locations and the involved carrier types of the CPs transitions are indicated in the energy band structure and projected density of states (PDOS).

2. Experiments

2.1. Sample preparation and characterization

High-quality HfS₂ single crystals were provided by Six Carbon Technology Shenzhen. These samples were prepared using the chemical vapor transport (CVT) method from high-purity raw materials and can be up to millimeters in size. The quality and elemental composition of the samples were confirmed via field emission scanning electron microscopy (FSEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) under ambient conditions. SEM photographs were taken using a field emission scanning electron microscope (Sirion 200, FEI Company, Netherlands). X-ray diffractograms were obtained using a commercial X-ray diffractometer (X'Pert3 Powder, PANalytical B.V.). And the X-ray photoelectron spectra were acquired by an X-ray photoelectron spectrometer (AXIS-ULTRA DLD-600 W, Kratos). Temperaturedependent Raman spectra were performed using a laser confocal Raman spectrometer (LabRAM HR800, Horiba JobinYvon) with a 532 nm laser over the temperature range of 100–600 K. The micro size range is ≤ 1 um using an 1800 gr/mm standard grating with a spectral resolution of 0.52 wavenumbers and a spectral repeatability of ± 0.2 wavenumbers. Heating and cooling rates were 50 K/min.

2.2. Temperature-dependent SE measurements

The HfS₂ sample was investigated utilizing an in-situ SE system that integrates a dual rotating compensator Mueller matrix spectroscopic ellipsometer (ME-L Muller matrix ellipsometer, Wuhan E-optics Technology Co.) with a vacuum variable-temperature system (see SI for the schematic diagram and experimental setup of the ellipsometer). The HfS₂ sample was placed on a precision thermal console (HCP621G-ELP, Instec Co.), sealed by a lid with three quartz windows (left side for incident light, right side for reflected light and top for a CCD camera) to form a vacuum chamber, and the temperature was monitored and adjusted by a temperature controller (mK2000, Instec Co.). During the measurement, a liquid nitrogen cooling device (LN2, Instec Co.) was used to cool the temperature to 100 K and the vacuum gauge reading was kept below 20 Pa. The heating rate was 130 K/min and the cooling rate was 50 K/min. The incidence angle of the SE measurement was set at 55° and the spectral energy ranges from 0.75 eV to 5.91 eV. The focal plane height was determined at room temperature, and remained no changed with the temperature since the sample was not moved, which ensure that the measurement point do not change during the variabletemperature SE experiments. Using a pair of focusing probes, the detected spot can be reduced to about 200 µm.

2.3. First-principles calculations

All calculations were performed with the Vienna Ab initio Simulation Package (VASP v6.3.0) [39]. The Perdew–Burke–Ernzerhof (PBE) functional of generalized gradient approximation (GGA) based on the projected augmented wave (PAW) pseudopotentials was used to describe the exchange correlation potential [40], and the Tkatchenko-Scheffler method with iterative Hirshfeld partitioning (TS/HI) [41] was applied to correct for Van der Waals interactions. In the optimization of geometric structure, we used the PBE functional based on PAW pseudopotential, with a kinetic energy cutoff of 500 eV and a $12 \times 12 \times 6$ Γ -centered k-point mesh. When calculating the projected density of states (PDOS), a denser $18 \times 18 \times 8$ Γ -centered k-point mesh was used. The convergence criterion of force was 0.01 eV/Å and of total energy was 10^{-5} eV. The effect of spin–orbit coupling (SOC) was considered in all calculations.

Frequency-dependent dielectric functions with and without local field effects (LFEs) were calculated using the GW60 and linear optics61 routines, respectively. Both calculations used a Γ -centered k-point mesh of 18 \times 18 \times 8, and the wave functions were computed with many additional empty bands, amounting to three times the number of self-consistent bands. The energy convergence criterion was set to 10^{-8} eV. LFEs were included at the level of the random phase approximation (RPA), considering only Hartree contributions. Converged LFEs were obtained using 266 G vectors.

3. Results and discussion

HfS₂ exhibits a typical van der Waals layered structure, belonging to the trigonal crystal system and the P3m1 space group, with lattice constants a = b = 3.69 Å and c = 6.61 Å [42]. As shown in Fig. 1(a), the in-plane directions are defined as the *a*-axis and *b*-axis, while the *c*-axis is oriented perpendicular to the *a*-*b* plane, extending outward. The *a*-*b* plane comprises a central Hf atomic layer flanked by S atomic layers on



Fig. 1. Schematic of HfS₂ crystal structure, front view (a), top view (b). (c) Field emission scanning electron microscopy image of HfS₂ sample surface magnified 1000 times. (d) X-ray diffractogram of the HfS₂ sample and a standard comparison card. X-ray photoelectron spectroscopy measurements of elements Hf (e) and S (f).

either side, forming a sandwich-like structure. Fig. 1(b) presents the top view of the a-b plane, clearly illustrating that each Hf atom is bonded to six S atoms, and each S atom is bonded to three Hf atoms. This arrangement results in a stable structure that exhibits in-plane isotropy. Fig. 1(c) displays the surface morphology of the HfS₂ sample, characterized by the FSEM. The sample surface is flat over a wide area, with only a few small grains present. Fig. 1(d) depicts the XRD patterns of the HfS2 sample with the reflection peaks identified at $2\theta \sim 15.03^{\circ}$, 30.42° , 46.53° , 63.62° , and 82.23° for the (001), (002), (003), (004), and (005) planes. In addition, the chemical composition of the HfS₂ crystal was further characterized by XPS, as shown in Figs. 1(e) and 1(f). Fig. 1(e) shows two peaks in binding energy (BE) at 15.65 eV and 17.3 eV,

corresponding to the Hf 4f7/2 and Hf 4f5/2 electronic states, respectively (for electrons with total angular momentum quantum numbers of 7/2 and 5/2 in the 4f orbital of Hf atoms). Similarly, Fig. 1(f) shows two peaks at 160.3 eV and 161.5 eV representing the S 2p3/2 and S 2p1/2 electronic states. These results are in good agreement with previous reports [43,44], demonstrating the high purity of the samples. All these characterization results indicate the high quality of the HfS₂ crystal, including the flatness and purity, providing a solid foundation for subsequent variable-temperature Raman and SE measurements.

Raman spectroscopy serves as an effective tool for probing phonon behavior in materials. Fig. 2(a) illustrates the Raman spectrum of HfS₂ as a function of temperature. It should be noted that for a clearer



Fig. 2. (a) Raman spectrum of HfS₂ samples at temperatures 100–700 K. Three Raman modes are labeled, where the inset illustrates the vibrational modes of two known modes. The three regions divided by dashed lines have different magnification factors, which are labeled below the image. SE-extracted real part (b) and imaginary part (c) of in-plane dielectric functions of HfS₂ sample at temperature 100–600 K. The gray part in the real part is negative, and there are seven critical points A–G marked in the imaginary part. Refractive indices (d) and extinction coefficients (e) of HfS₂ samples at temperatures of 100–600 K. The Ω and Λ points are the turning points.

presentation, the spectra are divided into three regions using dashed lines, and the signal strengths in these regions are magnified by different factors, with the corresponding magnification factors labeled below each region. Three main peaks are observed at 133.79, 257.69 and 335.22 \mbox{cm}^{-1} (all at 300 K), respectively corresponding to ω_1, E_g and A_{1g} Raman modes. The vibrational modes of Eg and A1g are demonstrated in the inset, while the origin of ω_1 has not yet been clearly established [29]. Our study focuses on the temperature dependencies of the E_g and A_{1g} . As the temperature increases from 100 K to 700 K, both modes exhibit a decrease in intensity and a broadening in the linewidth, indicating a significant enhancement of anharmonic effects and a reduction in phonon lifetime. In addition, the Eg model shows a clear redshift with the temperature increasing, in contrast to a blueshift below 300 K and a redshift over 300 K for the A1g model (see the Supplementary Material for results fitted with the Lorentz model). The redshift of the Eg mode is due to the reduction of the expected spring constant resulting from lattice expansion, which is a typical phenomenon. While the abnormal blueshift of A1g mode at low temperature is caused by the disproportionate thermal expansion behaviors between the thickness of the intralayer and interlayer in the multi-trilayer structure [45].

The SE is a powerful technique for determining the dielectric function of a material without imposing additional physical constraints [46–49], such as the Kramers-Kronig relationship. As a non-contact measurement method, the SE is widely utilized for analyzing nanomaterials and nanofilms. It can measure the change of polarization state before and after the interaction of polarized light with the sample, which is usually described by two ellipsometric parameters, namely the amplitude ratio angle Ψ and the phase difference angle Δ . The ellipsometric parameters are given by

$$\rho = \tan(\Psi)\exp(i\Delta) = r_p/r_s \tag{1}$$

where, i is the imaginary unit, ρ is referred to as the ellipsometric ratio, r_p and r_s denote the reflection coefficients of p-polarized and s-polarized light, respectively. For the ellipsometric analysis, an appropriate optical model and a parameterized dielectric model based on oscillators are initially constructed. Theoretical ellipsometric parameters are then calculated based on these models and fitted to the experimental ellipsometric parameters to ultimately determine the dielectric function. In the case of the tested sample, the optical model includes the HfS₂ crystal and an interface air/HfS2, while the dielectric model comprises one Gaussian oscillator, one Tauc-Lorentz oscillator, and six Lorentz oscillators to deal with the dispersion of HfS2 over the concerned spectral range [50,51]. When fitting the experimental data, the mean square errors (MSE) of the ellipsometric parameters are 3.423, 3.349, 3.195, 3.339, 3.592, and 8.433 for temperatures ranging from 100 K to 600 K. The MSE at 600 K are significantly higher compared to those at other temperatures due to the focal plane change caused by the lattice expansion at high temperatures, which results in an intensity decrease of the reflected signal received by the detector. It should be noted that to minimize the MSE at 600 K, the data exhibiting high noise at energies exceeding 5.5 eV were artificially truncated before fitting. The low MSE indicate a good agreement between the theoretical and experimental data, ensuring the correctness and accuracy of the obtained dielectric function. Detailed analysis procedures and results are provided in the ellipsometric analysis section in the SM. In our experiment, the optic axis of HfS₂ is oriented perpendicular to the sample surface, meaning that the incident light interacts primarily with the in-plane (ordinary) dielectric response. According to previous theoretical and experimental studies [52], under this specific configuration, the pseudodielectric function (PDF) measured by standard ellipsometry provides a good approximation to the actual ordinary dielectric function. Therefore, although the anisotropy in the out-of-plane direction is not explicitly included in our model, the extracted dielectric function still closely reflects the in-plane optical properties, which dominate the measured response on the van der Waals surface. As further evidence supporting

the validity of our in-plane dielectric function measurements, we also performed variable-incidence-angle ellipsometry at room temperature (shown in Fig. S4), which yielded consistent dielectric functions across different angles.

Figs. 2(b) and 2(c) show the real and imaginary parts of the in-plane dielectric function $\varepsilon = \varepsilon_r - i\varepsilon_i = (n - ik)^2$ of HfS₂ over the energy range of 0.75-5.91 eV under different temperatures as determined by SE, respectively. In Fig. 2(b), the real dielectric function ε_r is larger at low temperatures than that at high temperatures when the energy is lower than 1.988 eV, however, the exact opposite is true when the energy is larger than 1.988 eV. This turning point is labeled as Ω . In addition, the gray area in Fig. 2(b) represents regions of negative ε_r , which is associated with the bulk plasma resonance. By observing the intersection of the ε_r curve of HfS₂ with $\varepsilon_r = 0$, it is qualitatively determined that HfS₂ exhibits two plasma resonance frequencies. These can be analyzed more accurately by means of the electron energy loss spectrum (EELS) shown in Fig. S5. By looking at the EELS, there are two significant peaks at 2.95 and 4.19 eV, corresponding to the two plasma resonances. In Fig. 2(c), a total of seven CPs labeled with uppercase letters A-G can be observed. Each of them corresponds to a specific CP optical transition, parametrically described by the Lorentz or Tauc-Lorentz oscillator in the dielectric model. It should be noted that the Gaussian oscillator is usually introduced to deal with defect absorption or measurement errors in the SE analysis, without exact physical meaning. Thus, there is no observable CP corresponding to the Gaussian oscillator. Among them, CP B has a larger amplitude at low temperatures and CP D has a larger amplitude at high temperatures, while CP C is more special, which can be clearly observed at low temperatures and disappears gradually as the temperature increases. Figs. 2(d) and 2(e) respectively illustrate the refractive index n and extinction coefficient k of HfS₂. The temperature dependency turning point Λ in Fig. 2(d) occurs at 2.172 eV which is slightly larger than the energy location of Ω in Fig. 2(b). This is because in this energy range, k is larger at lower temperatures and n needs to have the same trend to ensure that the values of ε_r determined by the relation $\varepsilon_r = n^2 - k^2$ are equal at different temperatures. At these turning points, the real dielectric function ε_r or the refractive index *n* of HfS₂ is not affected by the temperature, which can be used to fabricate devices with stable performance at different ambient temperatures.

Fig. 3(a) shows the absorption spectrum of the HfS_2 sample with an absorption cut-off edge of 881 nm, implying a bandgap of 1.407 eV. This differs from previous studies and is attributed to the fact that the defects of the samples prepared by the different processes are not the same. The bandgap at the Γ point obtained from our first principles calculations is 1.018 eV shown in Fig. 5(a), which is lower than the experimental value, due to the fact that the PBE functional underestimates the bandgap value. The real part and imaginary part of dielectric function spectra of HfS2 were also obtained by first-principles calculations, which are shown in Fig. 3(b) and (c). It can be seen that the values of the in-plane dielectric function including LFE are closer to the experimental results in Fig. 2(b) and (c) compared to the in-plane dielectric function without LFE. And the similarity between the calculated and experimental results proves the correctness of the ellipsometric analysis. In addition, Figs. 3 (d) and (e) show the variation patterns of the four quantities ε_p , ε_b , n, and k with temperature, respectively. Here, two typical examples with significant patterns are chosen, where one set of data has energy values below the bandgap and the other has energy values above the bandgap. The trends are similar between ε_r and *n*, and between ε_i and *k*, which are determined by the inherent commutation relations between them. In Fig. 3(d), all four quantities decrease with temperature, and a review of Figs. 2(b-e) reveals that this is a common phenomenon below the bandgap. Variations of ε_r and *n* with temperature are mainly affected by physical processes, including thermal expansion, phonon excitation, and so on. In contrast, the variations of ε_i and k are more complex, with greatly enhanced contributions from defects and magazine states in addition to these physical processes [53]. Above the bandgap, these four



Fig. 3. (a) Reflected absorption spectrum of HfS₂. (b) Real part and (c) imaginary part of dielectric function of HfS₂ calculated including or not including local field effects (LFE). The change of dielectric function and complex refractive index with temperature when the energy is (d)1.227 eV and (e)2.782 eV.

quantities are affected by interband transitions, with trends varying with energies. Fig. 3(e) shows that ε_r and n increase with temperature because they are mainly dominated by CP B transitions at different temperatures.

these featured peaks with the temperature, a CP analysis of the dielectric function was carried out, which was realized by varying the CP parameters to fit the second-order derivative of the dielectric function with respect to the energy, which can be theoretically described by [54,55]

In order to more precisely investigate and discuss the evolution of



Fig. 4. Variation of amplitudes(a) and broadening factors(b) of CPs A–G with temperatures. (c) Variation of centre energies (black solid dots) of CPs A–G with temperatures and best-fit lines (red lines) fitted by Bose-Einstein model. (d) Structure of the 1T and 3R phases of HfS2. (e) Schematic diagram of the energy band structure with temperature change.

$$\frac{d^{2}\varepsilon}{dE^{2}} = \begin{cases} m(m-1)A\exp(\mathrm{i}\phi)(E-E_{0}+\mathrm{i}\Gamma)^{m-2}, \ m\neq 0\\ A\exp(\mathrm{i}\phi)(E-E_{0}+\mathrm{i}\Gamma)^{-2}, \ m=0 \end{cases}$$
(2)

where, A, ϕ , E_0 , and Γ denote the amplitude, phase, center energy, and damping coefficient of the critical points, respectively. The parameter m specifies the dimensionality of the CP optical transitions, and m = 1/2, 0, -1/2, and -1 respectively denote the three-dimensional, two-dimensional, one-dimensional, and zero-dimensional CP transitions. In the analysis of the SE-determined dielectric functions of HfS₂, m = 0 provided the best fit, indicating that these CPs are two-dimensional transitions associated with two-dimensional van Hove singularities, which are related to electron-hole interactions. All fitting results for $d^2 \varepsilon/dE^2$ for the CP analysis can be found in the SM.

Figs. 4(a) and 4(b) demonstrate the temperature-dependent evolutions of the amplitudes and broadening factors of CPs A-G. It can be seen that as the temperature increases, the amplitudes of CPs A, E, F and G slowly increase, while the amplitudes of CPs B, C and D notably decrease. The broadening factors of CPs B, C, E and G increase, while those of CPs A, D and F alternately decrease and increase with an overall insignificant trend with the temperature. These evolutionary trends are related to the increased thermal expansion effect of the lattice at high temperatures and the enhanced electron-phonon interactions. It should be noted that CP E disappears when the temperature is larger than 400 K, while the absence of CP G at 600 K is due to the truncation in the SE analysis. The behaviour of CP Cs and E is of interest, with a sharp increase in the broadening of CP C after 400 K as well as that of CP E after 300 K. Another manifestation of this behaviour is the gradual disappearance of the characteristic peaks of CP C, while CP E has disappeared after 400 K (see Fig. S6). According to previous reports, HfS2 undergoes a reversible phase transition from the 1T phase to the 3R phase after 300 K [45]. The structural transition is shown in Fig. 4(d). At the onset of the phase transition, CP E exhibited mutation. And when the phase transition occurs completely, i.e. after 400 K, CP C mutates and is accompanied by the disappearance of CP E. Fig. 4(c) gives the evolution relationships between the centre energies of CPs A-G versus the temperature, which can be fitted by the Varshni equation [56,57]

$$E = E_0 - \frac{\alpha T^2}{T + \beta} \tag{3}$$

or the Bose-Einstein model [58,59]

$$E = E_0 - \frac{2a_B}{\exp(\Theta_B/T) - 1} \tag{4}$$

where, E is the CP central energy at temperature T, E_0 is the central energy value at 0 K, α and β are constant parameters, β is related to the Debye temperature, a_B describes the electron-phonon interaction strength, and Θ_B denotes the average phonon temperature. For numerous semiconductors, the bandgap energy decreases with the temperature (i.e., exhibits a negative temperature coefficient), which can be well described by both models. However, there are also a large number of materials that display positive temperature coefficients, where α or a_B in the equation becomes negative, resulting in a loss of physical meaning. To more accurately describe these materials, it is necessary to modify the sign before the second term from '–' to '+' in both equations [60,61]. In Fig. 4(c), the center energies of CPs A-G all exhibit positive temperature coefficients, exhibiting a blueshift with increasing temperature. The reason for this change is explained in the schematic of Fig. 4(e). The bandgap E_g of HfS₂ consists of the exciton binding energy E_b and the optical bandgap E_o, where E_o corresponds to the center energy of the CP optical transition. As the temperature increases, both bandgap $E_{\rm g}$ and exciton binding energy $E_{\rm b}$ decrease, and the amount of change in optical bandgap E_o is equal to the absolute value of the difference between the decreases in E_g and E_b , i.e., $\Delta E_o =$ $|\Delta E_{\rm g} - \Delta E_{\rm b}|$. When the decrease in E_b is greater than the decrease in E_g,

 E_o increases and a blueshift occurs. And the red curves are fitting results using the Bose-Einstein model in Eq. (4), with the specific parameters shown in Table 1. The fitting results using the Varshni equation in Eq. (3) are shown in the SM. As can be seen from the Table 1, CP D and G have the smallest and largest electron-phonon interaction strength. Compared to other CPs, the electron-phonon interaction of CP C is not prominent, while its variation with temperature is the most notable, indicating that the lattice thermal expansion is the dominant influencing factor for CP C.

To estimate the effects of lattice thermal expansion, we calculated the dielectric function under different lattice strains, as shown in Fig. 5. In reality, the thermal expansion of the lattice is smaller than the strain values used in our calculations-even at 600 K, the a- and b-axes expand by only about 0.24 %, and the c-axis by approximately 0.2 % [34]. We also performed additional calculations using the thermal expansion coefficients to expand the lattice accordingly. However, we chose to present results for larger strains (1 %–6 %) in Fig. 5 because the trends in the dielectric function remain qualitatively consistent across this range, and the changes are more clearly visible. Our analysis again focuses on the imaginary part of the dielectric function, particularly the features associated with critical point (CP) transitions. Although the positions of the calculated absorption peaks differ from the experimental ones, a qualitative comparison is still meaningful. As shown in Fig. 5(b), the absorption peaks below 3.75 eV exhibit a blueshift with increasing lattice strain. CPs A-D fall within this range, with the shift of CP D being particularly pronounced, highlighting the significant impact of lattice thermal expansion. This observation is consistent with the weak electron-phonon interaction for CP D, as indicated by the low a_B listed in Table 1. In contrast, absorption peaks above 3.75 eV (CPs E-G) show an initial redshift due to lattice expansion. However, their overall behavior appears as a blueshift in the experimental data, which is attributed to the dominant influence of electron-phonon interactions-further confirming their large a_B .

The CPs originate from optical transitions between the valence and conduction bands in the energy band structure, which can be further analyzed using first-principles calculations. Figs. 6(a) and 6(b) present the calculated energy band structure and PDOS for HfS2, which can help to identify the locations of interband transitions in the Brillouin zone corresponding to the CPs, as well as the involved carrier types. CPs A, B, and E are situated between the high-symmetry points Γ and A. CPs A and B are located near the point Γ , in close proximity to each other, and correspond to optical transitions from V_2 to C_2 and from V_3 to $C_1,\,$ respectively. CP E, on the other hand, is associated with the transition from V_1 to C_3 . CP C is positioned near the point A and involves the transition from V₂ to C₂. CP D is found at the high-symmetry point M and corresponds to the transition from V_1 to C_1 . CP F is located at the point Γ between K and M, associated with the transition from V3 to C1. Additionally, CPs F and G are positioned between the points Γ -M and H-A, respectively, both corresponding to the transition from V₄ to C₁. The transition positions are also labeled in the PDOS shown in Fig. 6(b). The conduction band is primarily composed of Hf-5d orbitals, with minor contributions from S-2p and S-2 s orbitals. In contrast, the valence band is predominantly characterized by S-2p orbitals, though the contributions from Hf-5d and Hf-5p orbitals are also significant. Consequently, the transitions corresponding to CPs A-G are mainly associated with the

Table 1	
Fitting results for the CPs center energies by Bose-Einstein model.	

CPs\Paras	$E_0(eV)$	$a_B(meV)$	$\Theta_B(\mathbf{K})$
A	$2.788 {\pm} 0.000660$	47.6 ± 5.5	628.3 ± 46.3
В	$2.953{\pm}0.00125$	$\textbf{79.5} \pm \textbf{20.8}$	885.4 ± 123.0
С	$3.060 {\pm} 0.0106$	51.5 ± 40.9	$\textbf{374.8} \pm \textbf{236.3}$
D	$3.223{\pm}0.00107$	8.5 ± 4.2	$\textbf{380.5} \pm \textbf{148.4}$
E	$3.542{\pm}0.000471$	154.5 ± 4.0	449.3 ± 7.4
F	$4.956 {\pm} 0.0107$	$\textbf{28.4} \pm \textbf{28.1}$	$\textbf{265.2} \pm \textbf{229.4}$
G	$5.633 {\pm} 0.00817$	451.3 ± 223.6	916.8 ± 211.9



Fig. 5. (a) Real and (b) imaginary parts of the dielectric function calculated from first principles at 1 %-6 % lattice strain.



Fig. 6. Energy band structure(a) and projected density of states(b) of HfS₂ calculated based on PBE functional. The transition positions at CPs A–G are marked with arrows.

Hf-5d and S-2p states. Notably, at the initial points of the transitions in CPs F and G, the Hf-5d contributions in the valence band surpass those of the S-2p, indicating a strong correlation of CPs F and G with the Hf-5d state.

4. Conclusions

In conclusion, we have conducted a systematic investigation into the temperature dependence of the optical properties of HfS₂. By using Raman spectroscopy, we identified two Raman modes that behave in different ways, an Eg mode that is red-shifted with increasing temperature, and an A1g mode that is blue-shifted below 300 K and red-shifted over 300 K. Additionally, we precisely extracted the dielectric functions and complex refractive indices of HfS2 using the SE over a broadband energy range of 0.75 eV to 5.91 eV, across a temperature range of 100 K to 600 K. It is found that the HfS2 has two plasma resonances and two turning points where have temperature-independent real dielectric function or refractive index. Below the bandgap, both the real and imaginary parts of the dielectric function decrease with increasing temperature due to thermophysical processes, and defects and magazine states also lead to a decrease in the imaginary part. Whereas, above the band gap, the variation of the dielectric function is closely related to the interband transition behavior. By employing CP analysis, seven CPs labeled A-G were identified in the dielectric function spectra. With rising temperature, the amplitudes of CPs B-D decreased, while those of CPs A and E-G increased. Moreover, the broadening factors of CPs B, C, E, and G intensified, whereas the changes in the broadening factors of CPs A, D, and F were less pronounced. It is noteworthy that the broadening factors of CP C and E increase dramatically and eventually disappear after 300 K with the appearance of temperature-induced reversible phase transitions. The central energies of CPs A-G exhibited a general increasing trend, manifesting as a blueshift in the CP peaks, originating from the increase of the optical band gap due to the faster decrease of the exciton binding energy than the decrease of the band gap. These temperature-induced modifications can be attributed to lattice thermal expansion and electron-phonon interactions. The Varshni equation and the Bose-Einstein model describe well the blueshift of the central energies of CPs, giving the electronphonon interaction strength of these CPs transitions. Among the CPs, CP D exhibits the weakest electron-phonon interaction, while CP G displays the strongest. First-principles calculations further elucidate the locations in the Brillouin zone and the carrier types involved in the optical transitions corresponding to CPs A-G. This study underscores the strong temperature dependence of the optical properties of HfS2, offering valuable insights for optimizing HfS2-based devices or guiding the design of such devices across varying operational environments.

CRediT authorship contribution statement

Qihang Zhang: Writing – original draft, Visualization, Investigation, Formal analysis, Conceptualization. Honggang Gu: Writing – review & editing, Supervision, Methodology, Funding acquisition, Conceptualization. Zhengfeng Guo: Investigation, Formal analysis. Shiyuan Liu: Supervision, Project administration, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

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Data availability

The authors confirm that the data supporting this article have been included as part of the manuscript and the supplementary material.

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