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Enhancement of Lyman- α Emission for Detection of Diffracted Atomic Hydrogen Beams

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An attempt was made to enhance the Lyman- α emission for the detection of low energy atomic hydrogen beams diffracted from the surface by means of (1+2) resonantly enhanced multiphoton ionization (REMPI). Employing a Kr-Ar mixing cell, the efficiency of frequency tripling to generate the vacuum ultraviolet (VUV) emission around the Lyman α line was fairly enhanced by about one order of magnitude compared to that with an ordinary pure Kr cell. An ionization chamber filled with acetone was also investigated for the detection and monitoring of the VUV light. Monochromatic atomic hydrogen (H) beams were prepared either *via* photodissociation of hydrogen-bromine (HBr) molecules at 243 nm with de Broglie wavelengths of 0.31 Å and 0.25 Å, or *via* photodissociation of hydrogen-iodine (HI) molecules at 266 nm with de Broglie wavelengths of 0.35 Å and 0.23 Å, respectively. Employing these H-beams, feasibilities for detection and visualization of diffraction patterns from the surface by the use of a fast optical imaging system were investigated by means of computer simulation experiments.

1. Introduction

The most advantageous feature of the atomic beam diffraction, especially the use of an atomic hydrogen (H) beam, is one of the most ideal methods to obtain lots of valuable information about the "topmost monolayer" of the surface. Most diffraction methods, *e.m.*, an X-ray diffraction, an electron beam diffraction, or a neutron beam diffraction, are usually concerned with many surface atomic layers, and consequently the reciprocal lattice is commonly composed of discrete points in reciprocal-space, whereas in the case of the atomic H-beam diffraction all reciprocal lattice points on Ewald sphere come to satisfy the "Laue condition". It is really this point that makes the diffraction condition quite simple and easy to handle, when the atomic H beam was employed, comparing with other diffraction experiments.

In the previous papers, an improved scheme for atomic H-beam diffraction experiment was proposed¹⁾ and partly investigated,^{2), 3)} where a sufficiently intense monochromatic H-beam was prepared *via* two photolysis channels arising from parallel and perpendicular transitions of hydrogen-halide (HX) molecules. Here X includes bromine (Br) and iodine (I) atoms. An improvement of detection efficiency of diffracted H atoms was made by means of the (REMPI) technique with the aid of a tunable coherent vacuum ultraviolet (VUV) light around the Lyman α line.³⁾⁻⁶⁾ For detection of diffracted H atoms it may be desirable that the emission power of VUV light is as high as possible.

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Enhancement of Lyman α emission by about one order of magnitude was examined by the use of a Kr–Ar mixing cell instead of using an ordinary pure Kr cell. Intensity of Lyman α emission was monitored by the use of an ionization chamber filled with acetone vapor at a pressure of few Torr.⁷⁾ This acetone chamber was very useful and reliable for an intense VUV light showing a linear response over the wide range of the VUV emission power. The characteristic features of the acetone chamber will be described in some details.

The REMPI technique can be combined with the Doppler spectroscopy, when necessary for a measurement of, *e.g.*, a subtle inelastic process such as phonon scattering phenomena on the surface. Indeed, this detection scheme (referred hereafter as REMPI-Doppler spectroscopy) was proved to be very sensitive to provide even a “single-H-atom detection”.³⁾ For the detection and visualization of diffracted H-beam patterns, a fast optical imaging system was developed and examined previously with various experiments.^{8), 9)}

Fundamental features of all these schemes are seen in the previous paper in detail,³⁾ so in the following sections we will present only a brief description necessary for discussions of subsequent computer simulation experiments by which feasibilities of these schemes to the surface diffraction study are discussed.

2. Enhancement of Lyman α Emission

A VUV radiation around the Lyman α line was generated previously in a Kr cell by means of nonresonant frequency tripling of a fundamental UV laser around $\lambda = 364.5$ nm.³⁾ In the experiment the fundamental light was derived from a dye laser (Lambda Physik, FL2002) which was pumped with a Xe–Cl excimer laser (Lambda Physik, EMG 102). For an efficient third-harmonic generation (THG) to occur, it is essential that Kr gas is negatively dispersive, *i.e.*, Kr gas has a refractive index at the third-harmonic frequency less than its refractive index at the fundamental frequency.¹⁰⁾ The optimum

Fig. 1. Schematic view of the UV to VUV conversion system.

Fig. 2. A typical VUV conversion efficiency in the Ar-Kr mixing cell. The small peak around 80 Torr shows the local maximum obtained from the pure Kr cell. Ar gas was started to add from around 500 Torr to compensate the phase matching between the fundamental UV and the 3rd harmonic VUV.

Lyman α emission is obtained in proportion to the square of Kr pressure as far as the phase matching condition is satisfied. Indeed, Batishche *et al.*¹¹⁾ showed that the phase matching at $\lambda = 3648\text{\AA}$ and $1216\text{\AA}$ was able to obtain owing to the resonant transition at $1235.8\text{\AA}$.

However, an optimum conversion efficiency of the THG in the pure Kr cell breaks up with increasing input UV laser power by losing the phase matching relation between the third-harmonic and the fundamental laser waves.¹²⁾ The limitation caused by this intensity dependent changes of the refractive index can be enhanced efficiently by means of the phase matching by mixing with a positively dispersive rare gas. Usually a Kr-Ar mixed gas was employed.¹²⁾

Experiments were carried out to enhance the efficiency of UV to VUV conversion using the Ar-mixed Kr cell as shown in Fig. 1. The structure of the conversion cell was almost the same as employed in the previous experiment³⁾ except for a gas-handling

inlet with a piezoelectric valve to mix Ar gas and a fan to circulate better the mixing gas. The cell was first charged with pure Kr gas at a certain pressure, *e.g.*, 100 Torr. At around 100 Torr the output VUV emission reached to a maximum power. Then the output power gradually decreased and disappeared with an increasing pressure of Kr gas due to the failure of phase matching. Owing to the nonlinear property of Kr susceptibility, it is known that an conversion efficiency of the Lyman α emission higher than 10^{-5} is very hard to obtain.¹²⁾

Then Kr gas was stopped filling the cell around, *e.g.*, 800 Torr, and in turn Ar gas was carefully charged with the piezoelectric valve to compensate the phase matching relation between third-harmonic and fundamental waves. The output VUV emission began to increase again and was enhanced by about one order of magnitude as compared with those under pure Kr gas. A typical conversion efficiency curve showing the enhancement of VUV emission is demonstrated in Fig. 2. A full detail of the measuring scheme with an acetone chamber will be given in the next section. The total pressure to give the maximum VUV power was very sensitive to the mixing ratio of Ar to Kr gas, especially very steep at higher pressure side of the peak as seen from Fig. 2. So steady stable enhancement of the output power of the VUV emission was hardly possible to keep maximum beyond one order of magnitude, unless the circulation of the gas inside the mixing cell was performed with great care. Therefore, a moderate enhancement of the VUV power would be practical for an experiment where the steady VUV power is required.

A further increase of the emission efficiency would be obtained by the use of an ultra-pure gas which should raise the limitation caused by VUV absorption. Indeed, Langer *et al.*¹²⁾ improved the conversion efficiency by up to two orders of magnitude with a considerable effort to optimize the experimental conditions.

3. Detection of Intense Lyman α Emission

In order to detect the Lyman α emission, a VUV detector based on the ionization chamber filled with acetone vapor was employed.¹³⁾ An ordinary photon counting device such as a photo multiplier or a secondary electron multiplier³⁾ was inconvenient or unable to use for the present purpose, since their outputs were very likely to saturate when photons were gathered to a rather restricted area on the detector surface within a very short time interval. The situation can be overcome by the use of the acetone chamber because the principle is essentially based on the ionization chamber⁷⁾ in which no saturation of the output ionization signal is expected.

A cross sectional view of the acetone chamber is presented in Fig. 3. The chamber was a cylindrical structure essentially of the Kingdon cage,¹⁴⁾ and consisted of an outer electrode of 8 mm diameter and a central stainless steel wire of 1 mm diameter. The VUV light was introduced into the chamber through an MgF_2 window of 2 mm thick. The positive potential up to 500 volts was applied to the central wire with a vacuum-tight feed through. The acetone vapor was filled into the ionization chamber through a needle valve at a pressure of few Torr so as to absorb the VUV emission entering into the acetone chamber completely. The vapor pressure inside the acetone chamber was monitored with a pirani gage (ULVAC, GP-2T). The chamber was operated with the

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Fig. 3. Cross sectional view of the acetone chamber.

Fig. 4. (a) Power dependence of signals from the acetone chamber on the fundamental laser at acetone vapor pressure of 1 Torr. (b) Typical characteristic gains of the acetone chamber as parameter of acetone vapor pressure.

outer electrode at a negative potential with respect to the central wire. As the potential was raised above 100 volts, output signals from the chamber began to gain almost exponentially to about two orders of magnitude before the chamber became unstable. Ionization of acetone was considered to take place by absorbing one VUV photon, since the VUV power dependence of output signals from the acetone chamber was linear, *i.e.*, proportional to the cubic of the fundamental laser power as shown in Fig. 4a. The signal

gains due to gas multiplication were measured from 10 to 500 volts. Two signal-voltage characteristic curves for a fixed VUV emission intensity are shown in Fig. 4b for two typical acetone vapor pressures.

4. Preparation of Atomic Hydrogen Beam

A monoenergetic H-beam was prepared *via* photodissociations of parent HBr molecules at 243 nm¹⁾ and HI molecules at 266 nm.^{2), 3)} The photolysis at 243 nm was performed with the UV light from a dye laser (Lambda Physik, FL2002), and the photolysis laser at 266 nm was produced by the fourth harmonic light from a Nd : YAG laser (GCR-11, Quanta-Ray).

There are respectively two different photodissociation channels that are energetically possible at 243 nm for HBr molecules and 266 nm for HI molecules. One is the purely parallel transition to the $^3\Pi_1$ state dissociating to the ground H atoms and the spin-orbit excited X^* atoms: $[H(^2S_{1/2}) + X(^2P_{1/2})]$. Here X denotes Br or I atoms, respectively. The other is purely perpendicular transition to the $^3\Pi_0^+$ state dissociating to both the ground H and X atoms: $[H(^2S_{1/2}) + X(^2P_{3/2})]$. The photolysis geometry for extracting H-atoms produced by the perpendicular transition is shown schematically in Fig. 5. The photolysis geometry for H-atoms produced by the parallel transition is obtained by rotating the linear polarization plane of the photolysis laser by 90° around the injection axis. According to whether the photodissociation channel is parallel or perpendicular, recoiling H atoms have two distinct velocities: 1.27×10^4 m/s and 1.58×10^4 m/s for

Fig. 5. Photolysis geometry for the perpendicular transition.

Fig. 6. Experimental velocity data are fitted to the theoretical curve.

Fig. 7. Velocity distributions of H-beams for three different temperatures: 10 K, 150 K, and 300 K.

parent HBr molecules,⁸⁾ and 1.12×10^4 m/s and 1.75×10^4 m/s for parent HI molecules,⁹⁾ respectively. Details about the experimental geometries are described in the previous papers for HBr photolysis⁸⁾ and for HI photolysis.³⁾

As a typical example of the resulting H-beam produced *via* photo-dissociation of HI

molecules, velocity distribution data obtained experimentally through the perpendicular photolysis channel were fitted to the calculated curve for $T=300^\circ\text{K}$ in Fig. 6 showing the velocity spread of 2.3% at FWHM. Experimental velocity distributions for other three cases were also fitted well to the theoretical curves showing almost similar velocity spreads, *i.e.*, from 2.5 to 4.5%, though not shown in the figure. The monochromatic feature of H-beams with such a considerable intensity would be hardly obtained by the use of a conventional beam source with a mechanical velocity selector.^{15), 16)}

In the calculation of velocity distributions of recoiling H atoms, accurate knowledge about spectroscopic data, especially potential curves for both ground and excited states and corresponding vibrational wave functions were required. For simplicity we only consider here the perpendicular transition of HI photodissociation. Velocity distributions by other photodissociation modes can also be treated in the similar way. At room temperature ($\sim 300^\circ\text{K}$), only the vibrationally ground state is allowed, where a simple harmonic oscillator model is applied for the electronic ground potential of HI molecules. For an analytical repulsive curve dissociating to the ground hydrogen and iodine atoms, the potential function by Ogilvie¹⁷⁾ constructed from spectroscopic parameters of Huebert and Martin¹⁸⁾ is employed.

Then the resulting velocity distribution of recoiling H atoms $N(v)$ is given by summing up with respect to the rotational quantum number J of the parent molecule as³⁾

$$N(v) = N_0 \sum_J \exp[-M_{\text{HX}} \{(v - v(J))^2 / 2kT\}] \Psi_0(J)^2 f_{\text{rot}}(J), \quad (1)$$

where N_0 is the normalization constant, M_{HX} is the mass of the parent molecule, k is the Boltzmann constant, $\Psi_0(J)$ is the vibrationally ground state eigenfunction, $f_{\text{rot}}(J)$ is the rotational distribution function at the level J , and $v(J)$ is decided from the energy relation reflecting the rotational population of the parent molecule before excitation, respectively.

The velocity distribution was strongly dependent on the initial temperature of parent molecules. For the convenience of comparison, velocity distributions of recoiling H atoms photodissociated from parent HI molecules at different temperatures were calculated from Eq. (1) as shown in Fig. 7. Both experimental and calculational procedures were described in detail in the previous paper.^{1), 3)}

5. Simulation Experiment of Surface Diffraction

Computer simulations were carried out to investigate if the intensity and monochromaticity of the atomic H beam prepared *via* photodissociation of parent HX molecules are sufficient for studies of diffraction experiments. Simulations were also examined whether the present detection system with the use of the fast optical imaging device can provide a favorable experimental condition or not.

In the calculations of diffraction patterns from the surface, the following assumptions were made:

[1] The H beam is diffracted only from the topmost monatomic layer of a sufficiently cold surface. The (0 0 1) cleavage surface of LiF crystal (lattice constant: $2.84\text{\AA}$) is considered, unless otherwise stated.

[2] No beam width hitting the surface is taken into account in the actual calculation. The only requirement is that the experimental beam width should be sufficiently large compared with the lattice constant for the scattered wave vector $\mathbf{k}$ to be decided definitely.

[3] The velocity distribution along the beam direction is given by Eq. (1), while in the plane perpendicular to the beam direction is assumed Maxwell distribution which gives rise to an angular divergence of the beam.

Assumption [1] provides the most characteristic feature of the H beam diffraction compared to other type of diffractions such as the X-ray, electron beam, or neutron beam diffraction. In usual cases the diffraction occurs only when the reciprocal lattice point falls on the Ewald sphere satisfying the Bragg condition as

$$\mathbf{k} = \mathbf{k}_0 + \mathbf{G}, \quad (2)$$

where $\mathbf{k}_0$ and $\mathbf{k}$ are the wave vectors of the incident and scattered waves, and $\mathbf{G}$ denotes a reciprocal vector, whereas in the H beam diffraction the scattering occurs exclusively on the topmost monatomic layer. Consequently an ordinary three-dimensional reciprocal lattice becomes two-dimensional, *i.e.*, a "bundle of net rods" along the k_z axis passing through corresponding reciprocal net points in the k_x - k_y plane. Diffraction occurs everywhere the Ewald sphere intercepts these reciprocal net rods, satisfying the Laue condition as a result.¹⁹⁾ This is just the point where the H-beam diffraction makes the experimental condition quite feasible to perform.

A finite width of the incident beam considered in the assumption [2] to obtain definite $\mathbf{k}$ comes essentially from the requirement of the uncertainty principle. A beam width typically obtained in the experiment was 0.5 mm in diameter which of course satisfies above requirement for $\mathbf{k}$ and also the experimental requirement; the beam width should be sufficiently smaller than the diameter of the position sensitive detector (80 mm). It is the angle of divergence in the incident beam rather than the beam width that has an important effect on the resolution of the diffraction pattern.

Fig. 8. Experimental geometry used in the calculation of H-atom diffraction on (0 0 1) cleavage surface of LiF (lattice constant: 2.84Å).

Fig. 9. Typical diffraction patterns calculated for three different beam temperatures: (a) 10 K, (b) 150 K, and (c) 300 K.

Fig. 10. Typical diffraction patterns as a function of incident H-atom accumulation with a lower resolution by 1/4 as compared with that of temperature dependence (Fig. 9). (a) 1×10^4 atoms, (b) 5×10^4 atoms, and (c) 1×10^6 atoms.

Both angular divergence and velocity spread of the incident beam in the assumption [3] are attributed to the temperature of the parent molecule, and fairly essential to obtain the well-resolved diffraction patterns because the broad angular divergence and velocity distribution will produce diffraction peaks of large angular spread and consequently lead to a poor spatial resolution.

Taking account of these facts mentioned above, the experimental geometry employed in the calculations was chosen as follows: The incident H-beam comes along $\langle 110 \rangle$ crystal axis with the incidence and azimuthal angles of 45° and 0° , respectively. In Fig. 8, the diffraction geometry is shown schematically. The fast optical imaging detector, the effective diameter of which is 80 mm, is located at the position 150 mm apart from the diffraction point along $\langle 110 \rangle$ direction with the deflection angle of 90° . The diffraction patterns were mainly calculated for atomic H-beams produced by the photodissociation of HI molecules through the perpendicular transition with de Broglie wavelength of $0.35 \text{ \AA}$. Similar patterns were also obtained for H-beams of other three de Broglie wavelengths, *i.e.*, $0.23 \text{ \AA}$ for the parallel transition of HI molecules, and $0.31 \text{ \AA}$ through the perpendicular transition and $0.25 \text{ \AA}$ through the parallel transition of HBr molecules, respectively.

The diffraction pattern was calculated assuming the interaction potential $V(\mathbf{r})$ between incident H-atoms and surface atoms. The Morse potential in the z direction with a diperiodic condition in the (x, y) plane was employed using the same potential parameters of Finzel *et al.*¹⁶⁾ The exact expression of the diperiodic potential is given in Appendix. Typical diffraction patterns are demonstrated in Fig. 9 for three different temperatures of parent molecules corresponding to the velocity distributions in Fig. 7.

A well-resolved diffraction pattern up to 3rd order was obtained even for a beam at room temperature on the 80 mm display of the fast optical imaging device, where each pattern was accumulated by 10^5 atoms of incident H-beam.

Experimental applicability of the present fast optical imaging device was also examined concerning the sensitivity under the experimental conditions considered here by changing the number of incident H-atoms. The lowest detection efficiency of the device was calculated under the assumption that at least one H-atom would be scattered at the positions of highest order diffraction on the detector surface. This assumption was based on the fact that the present detection device was good for the "single-H-atom detection".³⁾ For comparison typical diffraction patterns calculated for three different intensities of the incident H-beam are demonstrated in Fig. 10 by lowering the resolution of the detector.

In conclusion, well-qualified monochromatic H beams with a sufficient intensity for surface diffraction experiments were obtained through the photodissociation of parent hydrogen halide HX molecules. By the enhancement of the Lyman α emission with the use of the Kr-Ar mixing cell, the detection system with the present fast optical imaging device was also proved to be sufficiently sensitive to the accumulation of incident H-beam as low as $\sim 10^3$ atoms.

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Appendix

The diffraction pattern I is calculated in terms of the structure factor $F_s(\mathbf{G})$ as given by

$$I = I_0 [F_s(\mathbf{G})/L^2] \quad (\text{A1})$$

with

$$F_s(\mathbf{G}) = (2\pi M_H/h^2) \int_{\text{cell}} V(\mathbf{r}) \exp(-i\mathbf{G}\mathbf{r}) d\mathbf{r}, \quad (\text{A2})$$

where I_0 is the intensity of the incident H-beam, L is the distance between the diffraction point and the detection point. Here we assumed the Bragg condition: $\mathbf{k} - \mathbf{k}_0 = \mathbf{G}$. The interaction potential between the incident H-atom and the surface $V(\mathbf{r})$ in the structure factor is a diperiodic function of the surface lattice and can be expanded generally with respect to the reciprocal lattice vector $\mathbf{G}$:

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_G(z) \exp(i\mathbf{G}\mathbf{R}), \quad (\text{A3})$$

with

$$\mathbf{G} = m\mathbf{G}_x + n\mathbf{G}_y, \quad |\mathbf{G}_x| = |\mathbf{G}_y| = G, \quad \text{and} \quad \mathbf{R} = (x, y),$$

where (m, n) is any combinations of integers, G is the reciprocal lattice constant, and $\mathbf{R}$ denotes surface lattice points, respectively.

The summation in Eq. (A3) can be restricted approximately to four nearest neighbors of the order of $(1, 0)$: $(\pm G, 0)$ and $(0, \pm G)$, and four second nearest neighbors of the order of $(1, 1)$: $(\pm G, \pm G)$. Considering the rotational symmetry of the surface, four expansion coefficients $V_G(z)$'s of the order $(1, 0)$ are all identical and we designate them to be V_{10} . Similarly we designate all four coefficients of the order $(1, 1)$ to be V_{11} . Then the interaction potential is approximated as

$$V(\mathbf{r}) \approx V_0(z) + 2V_{10}(z)[\cos Gx + \cos Gy] + 4V_{11}(z) \cos Gx \cos Gy. \quad (\text{A4})$$

The main term $V_0(z)$ in Eq. (A4) is conventionally chosen to be a Morse potential:

$$V_0(z) = D \{ \exp[2\kappa(z_m - z)] - 2 \exp[\kappa(z_m - z)] \}, \quad (\text{A5})$$

with the depth D ($=17.8$ MeV), the reciprocal range parameter κ ($=1.04 \text{ \AA}^{-1}$) and the coordinate of the potential minimum z_m ($=2.7 \text{ \AA}$). Other expansion coefficients, $V_{10}(z)$ and $V_{11}(z)$, are chosen to be exponentially repulsive:

$$V_{10}(z) = \beta_{10} D \exp[2\kappa(z_m - z)], \quad (\text{A6})$$

$$V_{11}(z) = \beta_{11} D \exp[2\kappa(z_m - z)], \quad (\text{A7})$$

using the same parameters as employed by Finzel *et al.*¹⁶⁾ to be $\beta_{10} = 0.055$ and $\beta_{11} = 0.027$.