Sensitivity of gas-phase electron diffraction images to the molecular potential parameters

Ngoc-Loan Phan\textsuperscript{1,*}, Hien T Nguyen\textsuperscript{2,3,4}

\textsuperscript{1}Ho Chi Minh City University of Education, Ho Chi Minh City, Vietnam
\textsuperscript{2}University of Science, Ho Chi Minh City, Vietnam
\textsuperscript{3}Vietnam National University, Ho Chi Minh City, Vietnam
\textsuperscript{4}Tay Nguyen University, Buon Ma Thuot City, Vietnam

E-mail: loanptn@hcmue.edu.vn

Abstract. The gas-phase electron diffraction (GED) is a conventional method to extract the geometrical structure and the vibration parameters of molecules. In practice, the mean vibration amplitude is retrieved successfully, while the anharmonicity parameter is usually fixed by a relation with the former. To explain the reason, we examine the sensitivity of the molecular scattering curve (\(sM(s)\)) of \(N_2\) molecule to the vibration parameters. The results show that the \(sM(s)\) curve is sensitive to the mean vibration amplitude but considerably stable with the changing of the anharmonic parameter even at a high temperature. Besides, many recent studies also focus on the investigation of the laser-induced electron diffraction (LIED) since its high temporal and spatial resolution. However, it is hard to extract the vibration parameters from the LIED data because of the shortage of the analytical form of \(sM(s)\) caused by the complicated physical process. So we propose to directly reconstruct the molecular potential instead of extracting the vibration parameters from the LIED. The preliminary purpose is to test the sensitivity of the \(sM(s)\) curve to the potential parameters of the Morse potential of \(N_2\) considering the nuclear vibration for GED. We demonstrate that the \(sM(s)\) curve is sensitive to the change of the potential parameters; thus, the molecular potential can be reconstructed from the GED. This statement is an essential precondition for further investigation of not only the influence of the vibrational effect on the probing of the molecular dissociation but also the reconstruction of the molecular potential from the LIED data.

1. Introduction

The gas-phase electron diffraction (GED) is one of the effective diffraction methods to retrieve the static molecular structure. From the GED data, the molecular structure is refined by the fitting algorithm of the experimental data with the theoretical one calculated for trial molecular-configuration \([1–10]\). However, the comparison between the experimental and theoretical cross section of the electron-molecule diffraction displays considerable discrepancy \([11, 12]\). Many studies have explained this discrepancy by the influence of nuclear vibration and the anharmonicity of molecules \([11, 13, 14]\). The nuclear vibration corrects the retrieved molecular parameters \([11, 13]\) or causes a shrinkage effect \([1, 14]\). Besides, considering the nuclear vibration, the vibration parameters of molecules are also extracted \([1–10]\) thanks to the analytical formula of the differential cross section (DCS) or the molecular scattering curve \((sM(s))\). In particular, the mean vibration amplitude is successfully retrieved while the anharmonicity parameter is
usually fixed by a relation with the former [1, 2, 5–7, 10]. Up to date, the conventional GED method is exploited to get the molecular structure of complex molecules [8–10].

However, the GED method is not convenient for probing molecular dynamics. Some alternative electron diffraction methods have been proposed, such as X-ray free-electron laser [15], or ultrafast electron-diffraction [16]. These approaches archive the temporal resolution to order hundreds of femtoseconds [15, 16], but still too long for molecular vibration, or molecular reactions whose time scale is about tens of femtoseconds or less. Another method is adopting the electron diffraction when molecules are exposed to an ultrashort intense infrared laser pulse, which is called laser-induced electron diffraction (LIED) [17–20]. The LIED can be understood by the three-step model [21], where firstly, electron is tunnel ionized into the continuum state; then, it is accelerated and accumulated energy in the laser field; finally, when the electric field reverses its direction, the electron is driven back and rescatters on the parent ion.

Thanks to the quantitative rescattering theory, the DCS can be extracted from the LIED spectra [17]. In turn, utilizing the DCS from the LIED data induced by mid-infrared laser, Blaga et al. revealed snapshots of N2 and O2 molecules during the dissociation [18]. In 2016, Wolter et al. extended to probe the departure of H+ from the [C2H2]2+ [20]. In 2017, we also investigated the extraction of the molecular structure, but for near-infrared intense laser [22]. However, in these above-mentioned studies [18–20, 22], the molecular vibration is ignored. It is desirable to extend these studies to consider the effect of nuclear vibration. Unfortunately, the analytical formula of sM(s) of the GED method no longer can be applied for LIED data since its complicated physical mechanism. In fact, in the LIED process, the ionization makes the neutral molecule transform to the molecular ion. Moreover, according to the Franck-Condon principle [23], the distribution of the vibration levels is changed. Latter, the nuclear wave packet undergoes a time evolution before the rescattering of the returning electron. Besides, the nature of electron-ion collision is much different from the collision on neutral molecules due to the existence of long-range potential [22]. Therefore, it is difficult to refine the molecular vibration parameters since the shortage of analytical formula of DCS as in the GED.

In principle, the vibration parameters are derived from the molecular potential. Therefore, we propose to directly extract the potential parameter adopting the numerical sM(s) curve, which includes all above mentioned physical processes in the LIED. Our long-term goal is the study the influence of the vibration effect on the snapshots of the molecular image during the dissociation, and also reconstruct the molecular potential from the LIED data. As a consequence, the preliminary but essential stage is to examine the sensitivity of the electron-molecule diffraction quantities to the potential parameters.

In this study, we evaluate the sensitivity of the electron-molecule diffraction images to the potential parameters. For simplicity, the test is performed for GED data, and the sensitivity of the LIED images should be similar. Firstly, we examine the sensitivity of the molecular scattering curve sM(s) to the vibration parameters of N2. This goal aims to thoroughly understand the reason that in practice, the mean vibration amplitude is successfully retrieved from the experimental data while the anharmonicity parameter is usually fixed or ignored [1, 2, 5–7, 10]. For systematically, the investigation under various conditions of electron collision energies and temperatures is analyzed. Then, we test the sensitivity of the numerical curve sM(s) to the parameters of the Morse potential considering the nuclear vibration.

The rest of the paper is organized as follows. Section 2 presents the Morse potential and the calculation method of the molecular DCS and sM(s). Section 3 shows our results and discussion. The paper finishes with a conclusion.

2. Theoretical method
For the further purpose of reconstruction of the molecular potential, we have to parameterize the anharmonic potential. The simplest one for a diatomic molecule is the Morse potential. In this
section, first, we describe the Morse potential and its analytical solutions following Refs. [24–26]. Then, the numerical and analytical method to calculate the electron diffraction images, such as the molecular scattering curve and the differential cross section, is presented.

2.1. Morse potential

The Morse potential has form

\begin{equation}
V(x) = D_e (1 - e^{-\alpha(x-x_e)})^2, \tag{1}
\end{equation}

where \(x\) is the interatomic distance; \(x_e\) is the equilibrium bond distance; \(D_e\) is the dissociation energy from the minimum in the potential well; \(\alpha\) is a parameter controlled the force constant and the anharmonicity. In this study, we use potential parameters for \(N_2\), with \(D_e = 0.364\) a.u., \(\alpha = 1.424\) a.u., \(x_e = 2.0749\) a.u., which are given in Ref. [27].

The Hamiltonian of a particle with reduced mass \(m\) in the Morse potential is

\begin{equation}
\hat{H} = \frac{\hat{p}^2}{2m} + V(x). \tag{2}
\end{equation}

The eigenvalues for vibration level \(n\) are written as

\begin{equation}
E_n = -D_e + \hbar \omega [(n + 1/2) - \lambda (n + 1/2)^2], \tag{3}
\end{equation}

where \(\omega = \alpha \sqrt{2D_e/m}\) is the fundamental frequency, and \(\lambda = \sqrt{2mD_e/\hbar \alpha}\) is the anharmonic constant. The normalized wave function has analytical form

\begin{equation}
\psi_n = N_n e^{-z/2} z^{b/2} L_n^b(z). \tag{4}
\end{equation}

Here,

\begin{equation}
N_n = \sqrt{\frac{a \cdot b \cdot n!}{\Gamma(k-n)}}, \tag{5}
\end{equation}

\begin{equation}
z = ke^{-\alpha(x-x_e)}, \tag{6}
\end{equation}

\begin{equation}
b = k - 2n - 1, \tag{7}
\end{equation}

\begin{equation}
k = 2\frac{2mD_e}{\hbar \alpha}. \tag{8}
\end{equation}

and \(L_n^b(z)\) is the associated Laguerre polynomial.

2.2. Independent atomic model and vibration effect

The simplest model to calculate the molecular diffraction images is the independent atomic model (IAM) [28], which works well at high collision energy. Within IAM, a molecular scattering amplitude is considered as a sum of the independent atomic ones with an additional phase

\begin{equation}
F = \sum_j f_j e^{-is \cdot R_j}, \tag{9}
\end{equation}

where \(F, f_j\) is the molecular and the complex \(j\)-atomic scattering amplitudes, \(R_j\) is the position vector of atoms, \(s = k - k'\) is the momentum transfer vector. The differential cross section (DCS) or \(|F|^2\) for a randomly distributed sample of molecules is given by

\begin{equation}
<I>_{tot} (\theta) = I_A + I_{mol}. \tag{10}
\end{equation}
where $I_A$ is an incoherent sum of the scattering cross section from all the atoms in the molecule. $I_{mol}$ is the molecular scattering intensity described the interference of atomic scattering waves from different atoms

$$I_{mol} = \sum_{i \neq j} f_j f_j^* \frac{\sin(sR_{ij})}{sR_{ij}},$$

(11)

in which $R_{ij} = |\mathbf{R}_i - \mathbf{R}_j|$.

In fact, the molecular vibration exists in the electron diffraction patterns. Under the nuclear vibration, the average molecular scattering intensity is defined as shown in Refs. [11, 13, 14]

$$I^v_{mol} = \int_{-\infty}^{\infty} P(x,T)I_{mol}(x)dx.$$  

(12)

For diatomic molecule, $x = R_{12}$. $P(x,T)$ is the probability distribution of the vibration level

$$P(x,T) = \sum_{n=0}^{\infty} f_n(T)|\psi_n(x)|^2,$$

(13)

where $f_n(T)$ is the Boltzmann distribution in the thermal equilibrium at temperature $T$.

Since the molecular structure parameters are relevant to the term of molecular scattering intensity only, thus to enhance the sensitivity to the molecular structure, a molecular contrast factor $M(s)$ is defined as given in Refs. [13, 14]

$$M(s) = \frac{I_{mol}}{I_A}.$$  

(14)

When multiplying $M(s)$ with $s$, we obtain the function $sM(s)$ called the molecular scattering curve. The Fourier transform of $sM(s)$ gives the radial distribution curve, which is much meaningful in the determination of the molecular structure. The peak position of the radial distribution curve shows the specific internuclear distance, while the width of the peaks represents the mean vibrational amplitude.

By approximately expanding the probability distribution function of the vibration level to the cubic oscillator, the $sM(s)$ function for diatomic molecule has the analytical form [13, 14]

$$sM(s) = \frac{2|f_1 f_2^*|}{I_A} e^{-l^2 s^2/2} \frac{(sr_a - s^3 \kappa)}{r_a}.$$  

(15)

Here, $l^2 = \langle x^2 \rangle = \langle x \rangle^2$ is the square of the mean vibrational amplitude; $\kappa = (\langle r^3 \rangle - 3 \langle r \rangle \langle r^2 \rangle + 2 \langle r \rangle^3)/6$ is the anharmonicity parameter; and $r_a = \langle r^{-1} \rangle^{-1}$.

3. Results and discussion

The influence of the vibration effect on the electron diffraction patterns for conventional GED is thoroughly investigated in many textbooks and articles [8, 11, 13, 14]. In this study, firstly, we examine the effect of the molecular vibration in the molecular scattering curve of diatomic molecules. Figure 1 presents the numerically $sMs(s)$ curves for $N_2$ molecule without and with considering the vibration effect at the collision energy of 1000 eV. When the molecular vibration is ignored, the $sM(s)$ curve harmoniously oscillates with changing of the momentum transfer $s$. This harmonic variation is obviously by the form of the Eq. (11). However, when the molecular vibration is taken into account, the peak amplitude of the $sM(s)$ curve exponentially decays with increasing $s$. This decay is caused by factor $e^{-l^2 s^2/2}$ in the Eq. (15). This impact of the molecular vibration in the $sM(s)$ curve is similar to the results obtained in the previous studies [8, 11, 13, 14].
Figure 1. The molecular scattering curve of N$_2$ molecule without (solid black curve) and with (dotted red curve) the vibration effect at incident energy 1000 eV at room temperature 300 K. When the molecular vibration is taken into account, the peak amplitude of the $sM(s)$ curve exponentially decays with the increasing of the momentum transfer.

3.1. Sensitivity of molecular scattering curve to vibration parameters
The clear signature of the molecular vibration in the diffraction images encourages one to extract from them the molecular vibration parameters besides the geometrical structures [1–8, 10]. The
geometrical and vibration parameters were refined by the fitting algorithm of the experimental data with the theoretical molecular scattering curve $sM(s)$ or the molecular contract factor $M(s)$. The mean vibration amplitude is successfully retrieved while the anharmonic parameter is usually ignored, or fixed by a relation with the mean vibration amplitude [1,2,5–7,10]. To thoroughly understand the reason, in this subsection, we look insight the sensitivity of the molecular scattering curve $sM(s)$ to the vibration parameters. Moreover, we investigate this sensitivity property under various conditions of electron collision energy and temperature. In recent LIED experiments [18–20], an intense laser with long-wavelength, up to 3100 nm is utilized. So, the energy of the induced electron can archive up to 1700 eV at collision time (for laser with intensity of $6.5 \times 10^{14}$ W/cm$^2$). In this paper, for GED, the in-range energy of collision electron from 100 eV to 1000 eV is chosen.

Figure 2 exhibits the response of the molecular scattering curve $sM(s)$ to the changing of vibration parameters $l^2$ and $\kappa$ of 20% in comparison with the equilibrium value. The analytical approach (Eq. 15) is adopted to calculate these curves for N$_2$ molecule with the collision energy of electrons of 1000 eV at room temperature 300K. The result (Fig. 2 a) shows that the curve $sM(s)$ is considerably sensitive to the square of the mean vibration amplitude $l^2$ at a large value of momentum transfer $s$. To assess the sensitivity of the $sM(s)$ with the changing of parameters, we introduce a quantity called the relative difference, which is defined as $\delta = |sM(s)(y - 20\%) - sM(s)(y)|/|sM(s)(y)|$. Here, $y$ is a parameter, i.e., $l^2$ or $\kappa$. For the collision energy of 1000 eV, the relative difference of the vibration amplitude $l^2$ is most significant at the last peak, which is equal to 9.12%. However, for small $s$, it is hard to recognize the renovation of the $sM(s)$ curve with the changing of $l^2$. Moreover, for low collision energy, the $s$ value is restricted by a low value; as a consequence, the sensitivity of $sM(s)$ can be insignificant. To verify this statement, we examine the sensitivity of the $sM(s)$ curve for the case of lower energies of the incident electron. Figure 3 demonstrates the relative difference at the last peak of the $sM(s)$ curve for the vibration amplitude $l^2$ as a function of collision energy. It is indicated that the relative difference monotonically grows with increasing collision energy. For low energy, the relative difference is small; for instance, 1.6% at 200 eV. As a consequence,
the change of the $sM(s)$ curve within the error of 20% of $l^2$ is insignificant. Therefore, for the further goal of retrieving the vibration and potential parameters from the diffraction image LIED, it would be better if we use an appropriate laser to ensure the sufficiently high energy of the laser-induced electron.

In contrast to the vibration amplitude $l^2$, as shown in Fig. 2b, the molecular scattering curve is considerably stable with changing of the value of the anharmonic parameter $\kappa$. The maximum relative difference, i.e., at the last peak, is 0.003%. This insensitivity can be understood because, at room temperature, the nuclei mainly stay at the ground state where the impact of the potential anharmonicity is negligible. To enhance the influence of the asymmetry of the potential, the nuclei are stimulated to vibrate at higher vibration levels by high temperature or other techniques. Now, we study the change the $sM(s)$ curve for $N_2$ molecule at “assumed” high temperature 1000 K and 5000 K when the energy of the incident electron of 1000 eV. However, even at these high temperatures, the $sM(s)$ curve is almost unchanged with $\kappa$. The calculation reveals the relative difference at the last peak is slightly increased with increasing temperature. In particular, their values are 0.011% and 0.56% for 1000 K and 5000 K, respectively. To illuminate this phenomenon, we calculate the population of the vibration states. For the case of 5000 K, the population is 0.72, 0.16, 0.06, 0.03 for the ground, the 1st, the 2nd, and the 3rd excited states, respectively. The nuclei still mainly vibrate at low vibration levels; as a consequence, the signature of the anharmonicity parameter in the molecular scattering curve is insignificant. Therefore, the $\kappa$ value is usually initially fixed or ignored while extracting the geometrical structure and the vibration parameters of molecules from GED data [1, 2, 5–7, 10].

3.2. Sensitivity of reduced molecular scattering curve to potential parameters

In the above subsection, besides the geometrical structure, the vibration parameter can be extracted thanks to the analytical form of the DCS, $sM(s)$ (Eqs. 12, 15) for conventional GED considering the vibration effect. However, this analytical formula no longer can be applied for LIED data since the complicated physical mechanism in the LIED. Therefore, it is hard to retrieve the vibration parameters from LIED. One solution is exploiting the numerical DCS and $sM(s)$ curve (Eq. 12) directly simulated from a parameterized molecular potential, which includes all physical processes in the LIED data. Moreover, the vibration parameters $l^2$ and $\kappa$ are derived from the original molecular potential. Therefore, it is desirable to retrieve the potential parameters of the molecule. Besides, the atomic potential was also reconstructed from the LIED pattern for multielectron atom [29]. Our long-term goal is the study the influence of the vibration effect on the snapshots of the molecular image at different times, and also reconstruct the molecular potential from the LIED data by taking the nuclear vibration into account. However, the preliminary but essential stage is to examine the sensitivity of the electron-molecule diffraction quantities to the potential parameters. For simple, the test is performed for GED data, and the sensitivity of the LIED images can be similar.

Figure 4 presents the response to the changing of the potential parameters of the molecular scattering curve of $N_2$ at room temperature 300K and incident energy of electron 1000 eV. The result is numerically calculated considering the nuclear vibration associated with the Morse potential. Fig. 4 demonstrates that the $sM(s)$ curve is sensitive to both potential parameters $D_e$ and $\alpha$ of the Morse potential. The maximum relative difference, i.e., at the last peak, equals 5.45% and 10.72% for changing of $D_e$ and $\alpha$ compared to the equilibrium values, respectively. These parameters control the damping of the $sM(s)$ curve with increasing the momentum transfer. The sensitivity is more noticeable at large $s$; thus, the retrieval procedure would be more accurate if one uses an appropriate laser to create electrons with sufficient large $s$. Moreover, the relative difference, as a result, the degree of sensitivity of $sM(s)$ curve to the potential parameters $D_e$ and $\alpha$ (Fig. 4) is comparable to the sensitivity to the mean vibration amplitude $l^2$ (Fig. 2a). Also, the $l^2$ is successfully extracted from the experiment data of GED:
Figure 4. The molecular scattering $sM(s)$ curve of $N_2$ molecule at incident energy 1000 eV at temperature 300 K with changing the parameters $D_e$ (a) and $\alpha$ of 20%. The $sM(s)$ curve is sensitive to the both parameters $D_e$ and $\alpha$. The relative difference at the last peak is 5.45% and 10.72% for changing $D_e$ and $\alpha$, respectively.

thus, the potential parameters can also be expected to retrieve successfully.

4. Conclusion
Using the independent atomic model, we both analytically and numerically calculate the molecular scattering curve $sM(s)$ of the $N_2$ molecule considering nuclear vibration. Firstly, we examine the sensitivity of the $sM(s)$ to the vibration parameters - the square of mean vibration amplitude $l^2$ and the anharmonic parameter $\kappa$ to reveal the reason why the $l^2$ is well extracted from the experiment data, while the $\kappa$ is usually ignored or fixed by a relation with the $l^2$. The results show that the $sM(s)$ curve is sensitive to the square of mean vibration amplitude $l^2$, especially noticeable for large values of the momentum transfer $s$. On the contrary, the $sM(s)$ curve is stable with the changing of $\kappa$, even at high temperatures. Therefore, it is possible to extract the mean vibration amplitude $l^2$ while it is hard to get the $\kappa$ parameter.

In practice, the retrieval is performed by applying the analytical formula to obtained the “trial” theoretical $sM(s)$ curve while fitting with the experimental data. However, this analytical formula of $sM(s)$ considering nuclear vibration does not work for LIED data since its complicated physical mechanism. Therefore, instead of extracting the vibration parameters, we propose to reconstruct the molecular potential from the LIED. It is necessary to examine the sensitivity of the $sM(s)$ curve to the potential parameters. The result shows that the $sM(s)$ curve is responded to the changing parameters $D_e$ and $\alpha$ of the Morse potential. In short, the molecular potential can be reconstructed from the GED. This conclusion is meaningful for our further investigation of the influence of the vibrational effect on the probing the molecular dissociation, and reconstruct the molecular potential from the LIED data.
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