Multiple scattering model considering the vibration effect

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Abstract.

The independent atomic (IAM) and the multiple scattering (MS) models are recently adopted to extract the molecular geometrical structures from the electron diffraction images, especially, in the laser-induced electron diffraction. In this study, firstly, we clarify the working range of the MS and the IAM models by comparing its diffraction images at various collision energies. We claim that the MS model is effective at low energy of incident electron while both MS and IAM models give similar results at high collision energy. Secondly, we successfully develop the MS model by numerically including the molecular vibration. By comparing with the diffraction patterns calculated within the IAM model at considerably high collision energy, we verify the accuracy of the developed MS model. We show that the diffraction curves simulated by the MS and IAM methods considering the vibration effect are consistent with each other. Moreover, the extracted interatomic distance from diffraction images well agrees with the initial input. This evidence proves that the MS model with the vibration effect is reliable.

1. Introduction

X-ray and electron diffractions are powerful tools for spatial imaging of the molecular structure. Among them, gas-phase electron diffraction (GED) has been used for a long time to extract the interatomic distance and the chemical bonding of the molecule [1–3]. To get high spatial resolution, a high-energy electron beam is applied to penetrate the molecule during the electron-molecule collision [1, 2]. However, the GED method is not suitable for probing of the transient molecules whose time scale is about hundreds of femtoseconds or less. To achieve such temporal resolution, new electron diffraction methods have been developed, such as X-ray free-electron laser [4] or ultrafast electron-diffraction (UED) [5]. However, its time scale is still too long for molecular vibration or molecular reactions which occurs in about a few femtoseconds. Recently, the laser-induced electron diffraction (LIED) is exploited to get time-resolved molecular structure due to the collision of laser-induced electrons by an ultrashort laser pulse [6–9]. From LIED data, the molecular dynamics can be probed such as the molecular dissociation [7] or snapshots of the proton departure from $[C_2H_2]^2^+$ [9].

The molecular structure is extracted from the experimental GED, UED, and LIED data by their fitting with the theoretical calculation for trial molecular-configuration [2, 7–19]. There are two main approaches to calculate the theoretical differential cross section (DCS) – $ab\text{~intio}$
[20, 21], and using approximate models [22–25]. While the ab initio methods give more exact results, using the model has an advantage in reducing the computational cost. Thus, the latter is more preferred in refining the molecular structure from the experimental data. The simplest model is the independent atomic model (IAM) which works well at high collision energy [3, 22]. Moreover, the IAM model is also applied to retrieve the geometrical structure [26], and to probe the molecular dynamics [7–9] from the LIED data obtained when the molecule interacts with a mid-infrared intense laser. For lower energy of incident electrons in GED, or when molecules are irradiated by a near-infrared laser in LIED, the multiple scattering theory (MS) is more effective [23–25]. In the MS model, Hayashi and Kuchitsu [23] analytically expanded the IAM model by adding the partially double-scattering term. In 2017, we analytically improved the MS model by covering full second-order scattering [25]. In practice, the IAM model is intensively applied in extracting procedure for the high collision energy of incident electron [7–9, 22, 26, 27] since its agreement with the experimental data. In our point of view, it is also necessary to verify the IAM model using the more rigorous and evolved model. Since the MS model [23–25] is an extended model of the IAM, so exploiting the MS theory to examine the accuracy and the working range of the IAM model is needed.

Besides, many studies have demonstrated the essential role of nuclear vibration and the anharmonicity of molecules [3, 27, 28] in the diffraction patterns. The molecular vibration and anharmonicity shift the extracted molecular structures and cause the shrinkage effect [10, 17, 27]. For the IAM model, the vibration effect is both numerically and analytically included in the calculation [3, 17, 18, 27, 28]. However, the IAM model is suitable only for high-energy electron collisions. For a low-energy region of incident electrons, the MS is worth to use. Moreover, to the best of our knowledge, including the molecular vibration in the MS model is seldom reported. Thus, it is essential to develop the MS model with the molecular vibration, which is much meaningful for extracting geometrical structures and vibration parameters from the GED, LIED data in the low-energy range of incident electrons.

We have two goals in this study. Firstly, we examine the IAM model by the MS one to clarify the working range of the MS and the IAM models. Then, we develop the MS model by numerically including the molecular vibration and verify its reliability. This investigation is an essential stage of our long-term purpose for extracting both molecular structure and vibration parameters or potential parameters from the LIED data in the low-energy range of incident electron induced by the near-infrared laser.

The rest of the paper is organized as follows. Section 2 presents the IAM, MS models for “frozen” molecules. Besides, the numerical inclusion of the vibration effect in these models are also exhibited. Section 3 shows our results and discussion. The paper finishes with a conclusion.

2. Theoretical method
In this section, we briefly present the IAM and MS models following Refs. [23–25]. The numerical inclusion of the vibration effect in these models is also described.

2.1. Independent atomic model
According to the IAM model, the scattering amplitude of a molecule is a sum of the atomic ones

\[ F = \sum_j f_j e^{-isR_j}, \]

where \( F, f_j \) is the complex molecular and the \( j \)-atomic scattering amplitudes; \( R_j \) is the coordinate of fixed \( j \)-atom and \( s = k - k' \) is the momentum transfer vector. The DCS for a randomly distributed sample of molecules is given by

\[ I_{tot} = I_A + I_{mol}, \]

(2)
with $I_A = \sum_i |f_i|^2$ is an incoherent sum of the atomic cross sections and $R_{ij} = |\mathbf{R}_i - \mathbf{R}_j|$. The second term

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

is the molecular interference term (MIT) which includes the molecular structure information.

2.2. Multiple scattering theory

Hayashi and Kuchitsu [23] expanded the IAM model by adding the partially double-scattering term and called the MS model. In 2017, we analytically improved the MS model by covering full second-order scattering [25]. Here, we briefly recall some main formulae.

The total molecular DCS in the MS model can be split into terms

$$I_{tot} = I_A + I_{SS} + I_{SD1} + I_{SD2} + I_{DD} + I_{DD1}.$$ (4)

In which, the term $I_{SS}$ describes the interference of the single scattering waves.

$$I_{SS} = \sum_{A \neq B} \langle f_A f_B^* e^{is\mathbf{R}_{AB}} \rangle.$$ (5)

Here, $I_{SS}$ is the MIT term of the IAM model (Eq. 3). $A$, $B$, $C$, and $D$ are denoted as the label of atoms. The $I_{SD1}$ is the interference of the single- and the double-scattering waves, that has one common atom

$$I_{SD1} = \sum_{A \neq B} \langle f_A f_B^* e^{is\mathbf{R}_A} + f_B^* e^{is\mathbf{R}_B} \rangle + c.c.$$ (6)

where $f_{AB}$ is the double-scattering amplitude that describes the scattering path that electron collides atom A, then atom B before leaving the molecule. The $I_{SD2}$ covers the interference between single- and double scattering waves, but have no common atom

$$I_{SD2} = \sum_{A \neq B \neq C} \langle f_A f_B^* e^{is\mathbf{R}_C} \rangle + c.c.$$ (7)

The term $I_{DD}$ is the incoherent sum of the double-scattering wave

$$I_{DD} = \sum_{A \neq B} \langle |f_{AB}|^2 \rangle.$$ (8)

The Hayashi and Kuchisu’s work [23] truncated the expansion (Eq. 4) by the $I_{DD}$ term. We improved the MS model by taking into account the term $I_{DD1}$ described the interference of double scattering waves [25]

$$I_{DD1} = \sum_{A,B \neq C,D} \langle |f_{AB} f_{CD}^*|^2 \rangle.$$ (9)

The explicit analytical expressions can be found in Ref. [25]. In short, the MS model extends the IAM one by adding the $I_{add} = I_{SD1} + I_{SD2} + I_{DD} + I_{DD1}$, i.e., considering the multiple scattering effect.
2.3. Vibration effect and retrieving the molecular structure

Many studies [3, 27–29] have shown that considering the vibration effect in the calculation of the molecule-electron diffraction images makes the theoretical results more consistent with the experimental data. The molecular DCS when taking into account the vibration effect [27, 28]

\[ I_{\text{tot}}^v = \int_{-\infty}^{\infty} P(x,T)I_{\text{tot}}(x)dx. \]  

(10)

For diatomic molecule, \( x = R_{12} \) is the interatomic distance. \( P(x,T) \) is the probability distribution of vibration levels

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

(11)

where \( f_n(T) \) is the Boltzmann distribution of the vibration levels at temperature \( T \). \( \psi_n(x) \) is the wave function of the nuclei vibrated at \( n \) level. In this study, \( \psi_n(x) \) is solved by the time-imaginary method [30] for the nuclei move in the potential energy curve (PEC) of \( \text{O}_2 \). The PEC is simulated using program GAUSSIAN03 [31]. The simulated molecule \( \text{O}_2 \) has an equilibrium distance of 1.23 Å.

Since the molecular structure-parameters are hidden in all terms in Eq. 4 except \( I_A \). Therefore, to enhance the quantity of the retrieving the molecular structure, a molecular contrast factor \( M(s) \) is proposed as [3, 28]

\[ M(s) = \frac{I_{\text{tot}}^v - I_A}{I_A}. \]  

(12)

The expression for the case of ignoring the vibration effect is similar, but use \( I_{\text{tot}} \) instead of \( I_{\text{tot}}^v \). When multiplying \( M(s) \) with \( s \), we obtain the molecular scattering curve \( sM(s) \). For IAM model, the expression for \( sM(s) \) with the inclusion of the vibration effect has analytical form [18]

\[ sM(s) = \frac{2|f_1f_2^*|}{I_A} e^{-r^2s^2/2} \frac{(sr_a - s^3\kappa)}{r_a}. \]  

(13)

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

The Fourier transform of \( sM(s) \)

\[ D(r) = \int_0^{\infty} sM(s) \sin srd s. \]  

(14)

is called the radial distribution curve or the radial distribution function. The \( D(r) \) is useful in extracting the molecular structure. The peak position reveals the interatomic distance of each pair of atom in a molecule, while the width of the peak expresses the mean vibrational amplitude.

3. Results and discussion

In this section, first, we justify the IAM model and clarify its working range by an extended model of IAM, i.e., the MS model, without considering the vibration effect. Then, the molecular vibration is included in the MS model, and the results are discussed.
Figure 1. The theoretical DCS calculated by IAM and MS models, and experimental data of molecule O$_2$ (upper row) scattered by electrons with collision energy of 50 eV (a), 200 eV (b) and 500 eV (c). The difference between DCSs calculated by IAM and MS model is presented in the lower row. For low collision energy, the MS model agrees with the experimental data better than the IAM. In the high-energy region of incident electrons, the discrepancy between IAM and MS curves is insignificant. The experimental data is given in Refs. [32, 33].

3.1. Diffraction images calculated by the independent atomic and the multiple scattering models

For justifying the IAM model, we compare the DCS of molecule O$_2$ calculated by the IAM with the results obtained by the MS model, and also verify by the experimental data. In this section, the vibration effect is ignored. The results are exhibited in Fig. 1a–c for various collision energies of incident electrons. It is pointed out that the higher collision energy is, the closer the DCS curves calculated by MS and IAM are. The difference between them, $\text{error} = \frac{(I_{\text{tot}}^{\text{MS}} - I_{\text{tot}}^{\text{IAM}})}{I_{\text{tot}}^{\text{MS}}}$, can be illustrated in the lower row in Fig. 1. For the low collision energy, 50 eV (Fig. 1a), the discrepancy between DCSs (Fig. 1d), which are simulated by IAM and MS models, is remarkable, especially, approximately 78% at the minimum. Moreover, the theoretical DCS within the MS model is more fitted with the experimental data than the simulated IAM curve, thus using the MS model gives more accurate results. In sort, at a low-energy region of the incident electron, the contribution of the high-order scattering is significant, and the MS model gives more effective to calculate the molecule-electron diffraction patterns. The similar conclusion for low collision energy was pointed out in our previous study [25]. Now we proceed with study to the higher energy range of the incident electron.

With higher collision energy, the two DCS curves are better fitted to each other (Fig. 1b,c). Figure 2 shows the maximum difference between the DCSs calculated by MS and IAM models. The maximum error between the two methods is about 13%, 10% and 8% for electron energy 200 eV, 230 eV, and 300 eV, respectively (Fig. 2). Moreover, the discrepancy between the two models rapidly reduces with the increasing of the collision energy. Besides, the theoretical curves are closer to the experimental data when increasing the collision energy electron. Thus, in the high-energy range of incident electron, the high-order scattering is suppressed by the single one.

For the purpose of retrieving the molecular structure from the diffraction images, the
Figure 2. The maximum error between the DCSs of molecule O$_2$ calculated by the IAM and MS models as a function of collision energy. The horizontal dash line shows the error of 10%. The discrepancy between the IAM and MS models reduces with the increasing of collision energy.

Figure 3. The molecular contract factor of O$_2$ calculated by IAM and MS models at collision energy of 50 eV (a), 200 eV (b) and 500 eV (c). The two models are consistent with each other at high collision energy.

molecular contract factor MCF or the molecular scattering curve $sM(s)$ are adopted more popular than DCS [7–10, 15, 16]. The reason is that the MCF and $sM(s)$ eliminate the atomic cross-section $I_A$, which does not conceal the molecular structure. In Fig. 3 and Fig. 4, we respectively present the MCF as a function of the scattering angle; and the $sM(s)$ depending
on the momentum transfer \( s \), computed by the IAM and the MS models for various collision energies. The suitability of MCF (or the \( sM(s) \)) curves computed by IAM and MS models with increasing the electron energy is similar to that of the DCS. Note that for the MCF and \( sM(s) \), not the amplitude, but the oscillation property of the MCF curve plays a decisive role in the reconstruction of the molecular structure. One can see that for collision energy of 50 eV (Fig. 3a, 4a), the behavior of the MCF and the \( sM(s) \) within the MS model much diverges from the curves caused by the IAM, especially at scattering angle \( 97^\circ \) - the position of the minimum in the DCS (Fig. 1a,d). This discrepancy is caused by the dominant contribution of the high-order scattering in the molecule-electron diffraction. For higher collision energy, the oscillation period of the MCF (Fig. 3b,c) and \( sM(s) \) (Fig. 4b,c) calculated by the two methods are consistent with each other.

Figure 4. The molecular scattering curve \( sM(s) \) of \( \text{O}_2 \) with and without considering the nuclear vibration, numerically calculated by IAM and MS model at collision energy of 50 eV (a), 200 eV (b) and 500 eV (c). The molecular vibration strongly affects the \( sM(s) \) curve at large value of momentum transfer \( s \).

In summary, we conclude that for a low-energy of collision electrons, the MS model gives a better fit with the experimental data in comparison with the IAM model. With collision energy 230 eV, the difference between DCSs calculated by the IAM and the MS models are about 10\%. From 230 eV, the difference is reduced, and the discrepancy between the two methods is hard to recognize. Thus, for low energy of incident electrons, one can adopt the MS model to calculate the theoretical diffraction patterns. While for the higher collision energy, the multiple scattering effect is minor contribute to DCS, so the IAM model is considerably accurate.

3.2. Multiple scattering model considering the vibration effect

In the above subsection, it is clear that one should use the MS instead of the IAM model in the low-energy range of incident electron. Thus, the development of the MS model that gains the vibration effect is needed.

In this study, we numerically plug the molecular vibration in the MS model. The results for the molecular scattering curve \( sM(s) \) within the MS model in two cases – without and with the vibration effect are shown in Fig. 4 for three different collision energies. The calculations for the IAM model are also presented (Fig. 4). It is indicated that the molecular vibration modifies the \( sM(s) \) curve of the “frozen” molecule. For the electron energy of 50 eV, the vibration lowers the peak amplitude of the \( sM(s) \) curve of the MS model. With higher energy,
the discrepancy between the curves without and with including the molecular vibration is more noticeable. Specifically, in comparison with the case of ignoring the vibration, when including one, the peak amplitude of the $sM(s)$ decays with increasing the momentum transfer $s$. Besides, the oscillating period is also changed at large $s$. Moreover, the degree of vibrational suppression in the $sM(s)$ curve of the IAM and MS models is similar. For more explicit, the $sM(s)$ curve for collision energy 2000 eV is demonstrated in Fig. 5a. In other words, the molecular vibration smears out the peaks of the $sM(s)$ curve at large $s$.

The including of the vibration effect into the MS model is meaningful in retrieving the geometrical structure, and the molecular vibration parameters (or the molecular potential-parameters), especially, in the range of low collision energy. In fact, the molecular interatomic distances can be straightforwardly obtained by the peak positions in the radial distribution curve $D(r)$. However, from the Eq. (14), the momentum transfer value should cover from 0 to the infinity. It is impossible for numerical simulation and experimental data. In practice, the $s$ value is truncated at specific $s_{\text{max}}$; thus, the extracted interatomic distance, as a consequence of the $D(r)$ curve, can be acceptable if the high value of $s_{\text{max}}$, i.e., high collision energy is used. Therefore, the reconstruction of the molecular structure form the radial distribution function $D(r)$ is adopted for high collision energy only. For a low-energy region in which the MS works, the molecular structure is refined by the fitting of the experimental data with the theoretical one calculated for trial molecular-configuration.

![Figure 5](image_url)

**Figure 5.** The molecular scattering curve $sM(s)$ (a) and the radial distribution function $D(r)$ (b) of O$_2$ with and without considering the nuclear vibration, numerically calculated by IAM and MS model at collision energy of 2000 eV. The $D(r)$ curves calculated by the IAM and MS models are consistent with each other.

Our further goal is retrieving the geometrical structure and molecular potential-parameters from the diffraction images using the MS model considering the vibration effect at low collision energy of incident electrons. For this purpose, at this stage, we need to be sure about the accuracy of the developed MS model. To clarify it, we extract the interatomic distance from the $D(r)$ curve at energy 2000 eV. We use such high energy because of twofold reason: (i) it guarantees a sufficiently high $s$ value to perform the $D(r)$ calculation (Eq. 14); (ii) one can use
the IAM as a reference method to examine the MS model since its consistency at high collision energy. Fig. 5b exhibits the $D(r)$ curve calculated by the IAM and MS models with and without the inclusion of the vibration effect. It is shown that without the molecular vibration, the peak position is at 1.230 Å, as same as the initial input simulated by the GAUSSIAN program. When the vibration is taken into account, besides the smearing out of the peak, the vibration shifts the peak to the position 1.237 Å due to the anharmonicity of the potential energy curve [3, 18, 27]. This value is consistent with the $r_a = < r^{-1} >^{-1} = 1.236$ Å of the initial potential. Moreover, the peak region in the $D(r)$ curves calculated by the two methods – IAM and MS, entirely meets each other. Thus, we conclude that our developed MS model including the vibration effect is reliable.

4. Conclusion
Using the IAM and MS models, we calculate the diffraction images for diatomic molecule O$_2$ scattered by electrons with various energy. Firstly, we justify the IAM model and clarify its working range by the MS model without considering the vibration effect. For low-energy, the discrepancy between the IAM and the MS model is significant. Moreover, the MS model is better fitted with the experimental data. At high collision energy, the two models are consistent with each other. Thus, the MS model should be adopted for theoretically calculate the diffraction images at low energy of incident electrons. At high energy, the IAM model can be utilized.

Secondly, we develop the MS model by numerically including the molecular vibration and verify its accuracy. The vibration effect distorts the molecular scattering curve $sM(s)$ of the “frozen” molecule. At high energy, with considering the vibration, the amplitude of the $sM(s)$ curve decays with increasing the momentum transfer while peaks smear out compared to the case of ignoring the molecular vibration. Besides, the $D(r)$ curve at sufficiently high energy calculated by the MS model is entirely consistent with the IAM’s one. Moreover, the extracted internuclear distance from the $D(r)$ well agrees with the initial inputs. We conclude that we successfully develop a reliable MS model by including the vibration effect, which is meaningful in retrieving the molecular structure from the GED or LIED data in low collision energy.

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