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Vibrational Dephasing and Energy Relaxation of Admolecules by Phonons

by

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An investigation is made of the vibrational dephasing of a diatomic molecule adsorbed on a surface. Explicit analytic forms for the rate of dephasing by phonons are derived. For comparison, an expression for energy relaxation is given which is appropriate for OH on SiO_2. It is found that the dephasing rate is considerably faster for this system than the energy relaxation rate. These conclusions are compared with the results of a recent experiment.

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VIBRATIONAL DEPHASING AND ENERGY RELAXATION OF ADMOLECULES BY PHONONS

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Abstract

An investigation is made of the vibrational dephasing of a diatomic molecule adsorbed on a surface. Explicit analytic forms for the rate of dephasing by phonons are derived. For comparison, an expression for energy relaxation is given which is appropriate for OH on SiO_2. It is found that the dephasing rate is considerably faster for this system than the energy relaxation rate. These conclusions are compared with the results of a recent experiment.

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1. Introduction

The ways in which molecular vibrations relax at surfaces are of considerable interest in dynamical studies, not least for investigating the possibility of bond-selective chemistry. Recently,[1] an experiment was reported which has for the first time directly measured the rate of vibrational energy relaxation of an adsorbed species (OH on SiO_2, $v=1 \rightarrow v=0$). Knowledge of the total width of the absorption line[2] then allows an estimate of the pure dephasing rate through the relation $1/T_2 = 2/T_1 + 1/T_2'$, where T_1 and T_2' are the energy and pure phase relaxation times, respectively. There are undoubtedly many relaxation pathways, including direct coupling of the molecular mode to the phonons and formation of electron-hole pairs.[3] Silica, however, is a substrate in which the latter mechanism can be effectively ruled out.

We advance here a treatment of pure vibrational dephasing of an adsorbed diatomic molecule, via direct vibration-phonon coupling. For the sake of comparison, we give an expression for a T_1 pathway appropriate for OH/SiO_2. The model involves an anharmonic oscillator (A-B) coupled through an anharmonic bond (S-A) to a linear chain of harmonic oscillators. We show that phase relaxation is about $10-10^2$ times faster for this system than energy relaxation, in broad agreement with experiment. We also find the coupling to low frequency librational modes to be unnecessary for explaining experimental results. In this regard we feel it worth emphasizing the advantages of a linear chain model when the admolecule is aligned end-on at the surface. The assumption is that the dynamics of admolecule and surface is dominated by the motion of the whole system in the z-direction. Such a model has recently been successfully applied to the study of the desorption of an adatom.[4] The incorrect notion, that a linear chain model is one-dimensional in every respect, is quite widespread. In

fact, the density of states, a quantity needed for the calculation of rate information, is obtained from a fully three-dimensional (Debye) treatment, in which the phonon modes are assumed to form an isotropic continuum. The only real assumption apart from this is that the molecular dynamics is dominated by motion in a particular direction. Provided this is the case, such models are expected to give the correct order of magnitude.

2. Model

The details of the model are as follows. The momentum and position normal coordinates of the diatom-surface system are denoted by (p_1, q_1) and (p_2, q_2). When the frequencies of the bonds are sufficiently different, the motion of the center of mass of AB relative to the surface may be identified as one normal mode, and the vibration of A relative to B as the other. Thus we may make the identities $q_1 = z$ and $q_2 = x$. We shall focus on these position coordinates for the Taylor expansion of the potential, although in fact the nonadiabatic terms due to p_1 and p_2 give contributions of a similar order of magnitude.[5] The first term, in the Taylor expansion of the interaction potential, which gives rise to pure dephasing (i.e., the leading term in the expansion which is diagonal in the vibrational mode of the admolecule) is the quartic $k_{22}x^2$ term.[6]

In the theory of spectral lineshape, the width of a line is given by the imaginary part of the Zwanzig memory tetradic $\langle T(\omega_{fi} + i\varepsilon) \rangle_{fi,fi}$,[7] where ε is an infinitesimal quantity and the transition is being made between the initial (i) and final (f) state of the system. This may be expanded in powers of the interaction Liouville operator. In the Markov limit (short memory, T is constant) and in first order, there are two kinds of term: one represents contributions to the linewidth from inelastic scattering out of levels f and i, the other represents elastic transitions. The latter are identified with the "pure dephasing" interaction and an associated rate $1/T_2'$ given by:[8]

$$\frac{1}{T_2'} = \frac{\pi}{\hbar^2} \sum_{\alpha,\beta} d_{\alpha\beta}(|\langle\alpha|V^{(b)}|\beta\rangle|^2 - \langle V^{(b)}\rangle^2 \delta_{\alpha\beta}) \Delta_{fi}^{(s)} \delta(\omega_{\alpha\beta}) , \tag{1a}$$

where the bath-system interaction is assumed to be of the Form $V^{(b)}V^{(s)}$, in obvious notation.

$$\Delta_{fi}^{(s)} = {}_m\langle f|V^{(s)}|f\rangle_m - {}_m\langle i|V^{(s)}|i\rangle_m \tag{2}$$

is the relative displacement of the levels i and f of the molecule due to the anharmonic interaction with the bath; d is the canonical density operator for the bath, which is assumed to be diagonal and therefore describes the bath at thermal equilibrium. The indices α and β represent entire states of the bath. Put another way, Eq. (1a) represents the thermally averaged rate of Rayleigh scattering of phonons by the system (admolecule).

On the other hand, the inelastic rates are given, in the Markov limit, by the Golden Rule expression:

$$\frac{1}{T_1} = \frac{\pi}{\hbar^2} \sum_{\alpha,\beta} \sum_{f} d_{\beta\beta} |\langle\alpha|V^{(b)}|\beta\rangle|^2 |V_{fi}^{(s)}|^2 \delta(\omega_{\alpha\beta}-\omega_{if}) , \tag{1b}$$

which is essentially the thermally averaged rate of phonon absorption and emission by the system.

In order to introduce the bath-system coupling, we first evaluate the dynamics of AB moving with respect to a frozen surface atom S (i.e., the surface is represented by an atom of infinite mass). The influence of the thermal fluctuations of the lattice is then introduced by allowing the surface to displace by an amount u, which is fluctuating with time. Moreover, the assumption of Markovian behavior implies u(t) is uncorrelated with u(t'), t≠t'. We replace z with z-u and express u in terms of a Fourier sum over the normal coordinates of the lattice:[9]

$$u(t) = \left(\frac{\hbar}{2NM}\right)^{1/2} \sum_{k} \omega_k^{-1/2} (a_k^\dagger e^{-i\omega_k t} + a_k e^{i\omega_k t}) , \tag{3}$$

where there are N atoms in the chain, each of mass M, and $a_k^\dagger, a_k$ are the creation and annihilation operators for mode k, which has frequency ω_k.

First, we consider the dephasing of a two-level molecule attached to a surface. By making a Taylor expansion of the interaction it is possible to pick out terms which contribute to the process of interest. The first term in the interaction which gives rise to pure dephasing is $k_{22} u^2 x^2$, and therefore

$$V^{(b)}{}_V{}^{(s)} = k_{202} u^2 x^2 \quad . \tag{4}$$

Here, the subscripts represent the degree of excitation of phonons, adbond and molecule, respectively. Substituting Eqs. (3) and (4) into Eq. (1a) yields

$$\frac{1}{T_2'} = \frac{\pi k_{22}^2}{4M^2 N^2} \sum_{k,k'} d_{\beta\beta} \left(|\langle \alpha| a_k^\dagger a_{k'} + a_k a_{k'}^\dagger |\beta\rangle|^2 - \bar{n}_k^2 \delta_{kk'} \right) \Delta_{10}^{(s)} \delta(\omega_k - \omega_{k'}) \quad . \tag{5a}$$

Here, $\bar{n}_k$ is the thermal average of n_k, and is equal to $(e^\theta - 1)^{-1}$, with $\theta = \hbar\omega_k / k_B T$.

Converting the sum to an integral gives

$$\frac{1}{T_2'} = \frac{\pi k_{22}^2}{4M^2 N^2} \Delta_{10}^{(s)} \int d\omega_k d\omega_{k'} \; \frac{\rho(\omega_k)\rho(\omega_{k'})}{\omega_k \omega_{k'}} \bar{n}_k (\bar{n}_{k'} + 1) \quad , \tag{5b}$$

where $\rho(x)$ is the density of modes of frequency x. We now invoke the Debye approximation, in which the phonon states of a solid form an isotropic continuum with a density of states given by $\rho(\omega_k) = \dfrac{3\omega_k^2}{\omega_D^3} N$, where ω_D is the Debye frequency of the solid. This yields:

$$\frac{1}{T_2'} = \frac{9\pi k_{22}^2}{5M^2 \omega_D^6} \Delta_{10}^{(s)} I \quad , \tag{6a}$$

where

$$I = \int_0^{\omega_D} d\omega_k (\bar{n}_k^2 + \bar{n}_k) \omega_k^2 \quad . \tag{6b}$$

In order to evaluate $\Delta_{10}^{(s)}$ in Eq. (6a), we take the states $|1\rangle_m$ and $|0\rangle_m$ to be states of a harmonic oscillator, when

$$_m\langle j|x^2|j\rangle_m = \frac{2j+1}{2\mu_{AB}\omega_{AB}}\hbar \tag{7}$$

Here, μ_{AB} is the reduced mass of the admolecule and ω_{AB} its fundamental frequency. Moreover, we can define two limiting cases for which analytic solutions to Eq. (6b) are possible. In the limit of low temperature, $\theta \gg 1$, and ω_D may be taken to be infinity. In the limit of high temperature, $\theta \ll 1$ and the exponentials in the expression for $\bar{n}_k$ may be expanded, while retaining only the first term. Then we arrive at the following equations for the pure dephasing rate:

$$\frac{1}{T_2'} = \frac{3\pi^3 k_{02}^2 k_B^3}{4\hbar M^2 \mu_{AB}^2 \omega_{AB}^2 \omega_D^6} T^3 \qquad\qquad k_B T \ll \hbar\omega_D \tag{8a}$$

$$\frac{1}{T_2'} = \frac{9\pi k_{02}^2 k_B^2}{4 M^2 \mu_{AB}^2 \omega_{AB}^2 \omega_D^5} T^2 \qquad\qquad k_B T \gg \hbar\omega_D \tag{8b}$$

Consider now the energy relaxation of A-B. In the case of OH/SiO_2, $\omega_D = 340$ cm^{-1}, $\omega_{AS} = 970$ cm^{-1} and $\omega_{AB} = 3700$ cm^{-1}. Therefore, the first important interaction giving rise to energy relaxation is the sextic term, $(z-u)^5 x$, and in particular $uz^4 x$ which destroys one phonon, creates four quanta of adbond excitation and destroys the quantum of vibrational excitation in OH. Moreover we note that a direct one phonon deactivation of AB is not allowed by energy conservation, and that it would require at least eleven phonons.

We now identify eigenstates of the system as products of adbond states and molecular states. Using Eq. (1b) together with the Debye density of states yields

$$\frac{1}{T_1} = \frac{3\pi\gamma^2}{2M\hbar\omega_D^3}\bar{n}(\omega_p)\omega_p\,\Theta(\omega_p-\omega_D) \quad, \tag{9a}$$

where

$$\gamma = k_{141\ a}\langle 4|z^4|0\rangle_{a\ m}\langle 0|x|1\rangle_m \quad , \tag{9b}$$

and $\omega_p = 4\omega_{SA} - \omega_{AB}$; k_{141} is the coefficient of uz^4x. For simplicity we have taken the eigenstates of the adbond to be harmonic oscillator states. This is clearly a cruder approximation than making AB harmonic, especially given the level of excitation of SA (four quanta). However, there is little detailed information about the silica-hydroxyl bond, and we are in any case interested only in making an estimate of the rate of energy relaxation for this system. The introduction of anharmonicities into the SA bond will make the calculation only slightly more complicated. (Clearly, the interaction Hamiltonian depends only on the anharmonicity of the bond!)

It remains to determine k_{202} and k_{141}. Obviously, we must here take a proper account of the anharmonicity of the adbond, SA; indeed we shall make the assumption that this is the principal contributor to the coupling between the adbond and the molecular band AB. The validity of this assumption will be assessed at a later time.[10] Further we make the assumption that z, the distance between the surface and the center-of-mass of AB, is given approximately by the distance SA. This assumption is expected to be reasonable when A is must more massive than B (as in OH). Therefore, the motion of the AB bond gives rise to a modified Morse potential for SA in which the distance parameter is $z-\sigma x$, where σ is the ratio (M_B/M_A). A simple expansion of the Morse potential around the equilibrium distance then gives terms containing various combinations of powers of z and x. We are interested in the coefficient of the terms z^2x^2 and z^5x. Next we replace z with z-u and pick out the coefficients of u^2x^2 and uz^4x. We obtain finally

$$k_{202} = \frac{35}{6} a^4 \sigma^2 D \qquad \qquad (10a)$$

$$k_{141} = \frac{31}{18} a^6 \sigma D , \qquad \qquad (10b)$$

where a is the strength parameter of the AS Morse potential and D is the well depth. The parameter a may be written as $(\mu_{AS}/3D)^{1/2}$. To the best of our knowledge, D is an unknown quantity for OH/SiO_2, but we shall take it to be 1 eV, noting that both energy and phase relaxation depend upon D^{-2}. Thus changing D by a factor of 2 will result in a change in rate of a factor of 4. Finally, we use a Debye temperature for SiO_2 of 485 K and take the molecular weight, M, of the SiO_2 unit cell to be 60. From Eqs. (8a) and (9a) we now obtain $T_2' = 4ps$ and $T_1 = 2 \times 10^4$ ps, corresponding to widths of 1.3 cm^{-1} and 2.6 x 10^{-4} cm^{-1}, respectively. It is immediately clear that the calculated value for T_1 is about two orders of magnitude larger than the experimental value.[1] However, the value of T_2' is in much better agreement with the available information on this system,[11] where it is believed that the pure dephasing width ≤ 1 cm^{-1}.

The large discrepancy between the observed and calculated values of T_1 is very interesting, particularly since one of the approximations involved the assumption of a harmonic adbond for the calculation of k_{141} in Eq. (9b). Removal of this assumption will undoubtedly increase the estimate of T_1 still further. It is unlikely that the approximation either of the Debye model or of the linear chain dynamics are very important here. Of much greater importance is the crudity of our use of a Morse potential to estimate anharmonicities, particularly as (for T_1) the relevant terms are sextic.

However, the discrepancy is sufficiently large that we may tentatively postulate a different mechanism for the energy relaxation. The reason the mechanism given here leads to such long relaxation times is that the vibrational

quantum of the molecular bond is so large that energy transfer requires several quanta of excitation of other modes, and this is a process requiring at least a sextic anharmonicity. The _direct_ excitation of the substrate requires at least eleven phonons and may be presumed to be insignificant. It is possible that the OH couples to another kind of high-frequency mode, such as the Si-OH bend, although this mode is likely to be of a somewhat lower frequency than the Si-OH stretch we have considered. An interesting possibility is the direct energy exchange between adjacent hydoxyl groups on the surface. Even for weak coupling, such a pathway may be favored because the vibrational energy mismatch is zero. However, the irreversibility of energy relaxation demands several adjacent, anharmonically-coupled hydoxyl groups. In this regard, therefore, it will be interesting to see if T_1 increases with decreasing coverage.

As far as pure dephasing is concerned, the influence of an adjacent hydroxyl may be crudely modelled in terms of a dipole-dipole interaction.[13] Since the dipole moment depends upon vibrational state, such an interaction gives rise to a relative displacement of vibrational levels, which leads to a dephasing. For H_2O the vibrational dependence of the dipole is known and the dephasing contribution at room temperature may be estimated to be about $.01$ cm^{-1}. Assuming things are similar for OH, we can therefore rule out this contribution to the pure dephasing, since the calculated phonon-mediated contribution is two orders of magnitude faster. The calculation of the contribution of this admolecule-admolecule interaction to energy relaxation is less straightforward, and will be possible only when the anharmonic interaction between adjacent hydroxyl groups is known. It is also possible that the k_{141} term is much larger than our estimate, so that energy exchange with the lattice is important. Definitive answers await further experimental information.

During preparation of this manuscript we become aware of a recent paper by Persson,[12] which is similar in spirit to the present work. There a comparison

was made between energy relaxation and dephasing of the _adbond_, specifically for CO on nickel. The present work, on the other hand, describes relaxation of the molecular bond. Moreover, we have for the first time presented explicit analytical forms for T_2'.

Conclusion

We have derived expressions for pure vibrational dephasing and for vibrational energy relaxation of a diatomic molecule on a surface. The model involves the coupling of the molecular mode to bulk phonons. This is given in terms of the anharmonicities of the molecular and admolecular vibrations. By making an estimate of thee quantities for OH on SiO_2, we have shown that the prediction of the pure vibrational phase relaxation is in agreement with available experimental information, but the energy relaxation rate is two orders of magnitude smaller than experiment. This indicates the possibility of another mechanism in this case, and the obvious candidate is energy transfer between adjacent hydroxyl groups. A definitive answer will not be possible until the anharmonicities are known accurately. The influence of surface phonons will be assessed at a later time.[10] The inclusion of such modes is expected to be important for molecules lying across the surface as opposed to end-on, as in the present case. This is because of the expected efficient coupling between the lateral motion of the surface atoms and the motion of the molecular bond.

Acknowledgments

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11. T_1 is determined as 150 ps in reference 1. The experimental linewidth of 4-8 cm^{-1} (corresponding to 1.3-0.65 ps) for OH at the silica/vacuum interface is known to have an inhomogeneous component. Therefore, this must represent an upper bound on the dephasing contribution (J. C. Stephenson, private communication). It is believed that the width due to dephasing is ≤ 1 cm^{-1}, which corresponds to $T_2' \geq 5$ ps. Regarding our use of the low temperature formula when the temperature is actually a significant fraction of the Debye temperature (61%): we estimate that this will result in a slight (~20%) positive error in the calculation of the pure dephasing rate. Hence our estimate of ~ 1 cm^{-1} should be regarded as an upper bound.

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