

Coupled Modes Theory of Damped Harmonic Oscillator and Analysis of KDP Raman Spectrum

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The coupling of two low frequency modes with large dampings often plays an important role in the structural phase transition of crystals. A KDP crystal is a typical example. However, there seems to be much confusion as to the interpretation of the Raman spectra. In this paper we study the coupled modes theory^{1, 2)} to extract the correct physical information.

The general form of the equations of motion with a coupling can be obtained from Lagrange equation³⁾ including not only potential (U) but also dissipation energy⁴⁾ (D) assumed in the same forms as follow;

$$U = \frac{1}{2} K_{11} x_1^2 + K_{12} x_1 x_2 + \frac{1}{2} K_{22} x_2^2, \quad (1)$$

$$D = \frac{1}{2} \Gamma_{11} \dot{x}_1^2 + \Gamma_{12} \dot{x}_1 \dot{x}_2 + \frac{1}{2} \Gamma_{22} \dot{x}_2^2. \quad (2)$$

The directions of principal axes of U and D do not generally coincide with each other as shown in Fig. 1. Therefore, there is no unique way for the choice of the phase of the coupling constant. The important parameters describing the characteristic of the coupled system are poles ($\tilde{\omega}_{1,2}^d$) of the susceptibility $\chi(\omega)$. They do not depend on the coupling phase and can be obtained from the equation;

$$(K_1^i - i\Gamma_1^r \omega - \omega^2)(K_2^i - i\Gamma_2^r \omega - \omega^2) = 0 \quad (3)$$

where $(K_{1,2}^i)^{\frac{1}{2}}$ and $\Gamma_{1,2}^r$ denote the eigenfrequencies with the imaginary coupling constant and the damping factors with the real coupling constant, respectively. When $\chi(\omega)$ is decoupled, i.e., written as the sum of two independent modes with two poles ($\tilde{\omega}_{1,2}^d$), each mode is not represented by a damped harmonic oscillator (DHO) but has a form similar to the generalized Van Vleck-Weisskopf-Fröhlich susceptibility which has been derived before.⁵⁾

The results of the coupled modes analysis of KDP Raman spectrum are shown in Fig. 2 together with the results of a single overdamped mode analysis and of Debye formula analysis.⁶⁾

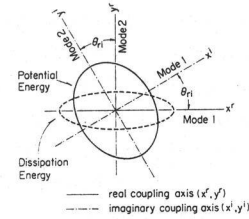


Fig. 1. Quadratic curves of potential and dissipation energy densities. Note that directions of principal axes are different each other.

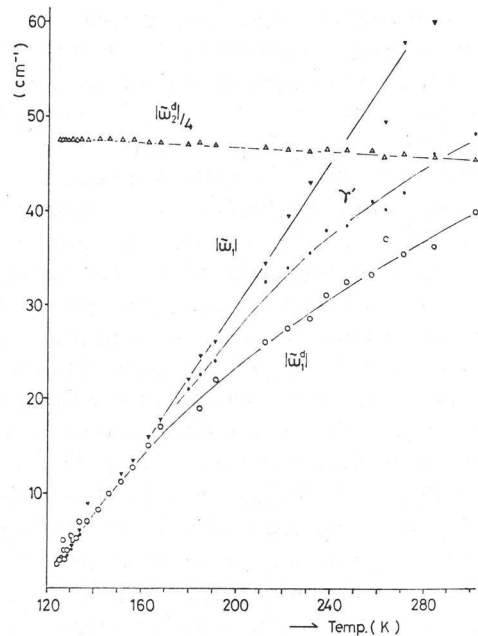


Fig. 2. Temperature dependences of absolute values of $\tilde{\omega}_{1,2}^d$ determined from eq. 3, $\tilde{\omega}_1$ of DHO and γ of Debye formula. See ref. 6.

References

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