

Ultrasonic attenuation and exchange striction in rare-earth metals

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A mechanism recently proposed by Vigren for explaining the anomalous field dependence of ultrasonic attenuation in rare-earth metals is shown to be equivalent to the exchange modulation mechanism phenomenologically proposed earlier. The explicit expression for the spin-phonon interaction in rare-earth metals is derived.

Acoustical attenuation in the paramagnetic region of heavy-rare-earth metals is strongly enhanced by application of a magnetic field.¹⁻³ For explaining this anomalous field dependence, the authors proposed the following mechanism.^{1,2,4} The longitudinal sounds are coupled with the local 4*f* spins through sound modulation of the indirect exchange interaction; the enhancement of the attenuation originates from the cross effect of the magnetization induced by the field and the spin fluctuation. Later, the authors formulated the attenuation in rare-earth metals as well as in itinerant magnets from the microscopic point of view.^{5,6}

Vigren has proposed the following mechanism to explain the field dependence of the attenuation mentioned above in a recent article.⁷ A magnetic field induces the polarization of the local 4*f* spins and this polarization splits the conduction spin subbands through the *s-f* exchange interaction. Repopulation of electrons in the spin subbands produces a spin polarization in the electronic density of states at the Fermi level; in this case, through the *s-f* exchange interaction, the thermal fluctuation of the local 4*f* spins can carry the charge fluctuation of conduction electrons along with their spin fluctuation; through this charge fluctuation, the fluctuation of the local 4*f* spins is coupled with the impressed sounds. Vigren claimed that this spin-phonon coupling mechanism is more important for the field dependence of the attenuation than the exchange modulation mechanism mentioned above. At first sight, Vigren's mechanism looks different from the exchange modulation mechanism. However, the fact is that both are the same. In this paper, we would like to show this point and to give the explicit expression for the spin-phonon interaction in the rare-earth metals.

Let us first introduce the *s-f* exchange Hamiltonian,

$$H_{sf} = -IN_0^{-1} \sum_k \sum_{k'} \sum_n \exp[i(\vec{k} - \vec{k}') \cdot \vec{R}_n] \times [S_n^z (a_{\vec{k}'}^\dagger a_{\vec{k}} - a_{\vec{k}}^\dagger a_{\vec{k}'})]$$

$$+ S_n^+ a_{\vec{k}'}^\dagger a_{\vec{k}} + S_n^- a_{\vec{k}}^\dagger a_{\vec{k}'}], \quad (1)$$

where $a_{k\sigma}$ is the annihilation operator of the conduction electron with wave number \vec{k} and spin σ , \vec{S}_n is the operator of the 4*f* spin at the atomic site \vec{R}_n , I is the *s-f* interaction constant, and N_0 is the number of the atoms in unit volume. The *z* axis is taken as the quantization axis of spins. We regard the *s-f* exchange interaction (1) as a perturbation Hamiltonian. The spin polarization of the conduction electrons is induced through the *s-f* exchange field (we neglect the direct effect of the applied field on the conduction electrons because it is negligible compared with the *s-f* exchange field). The free energy of the system is expanded in terms of the *s-f* exchange interaction. The first-order term vanishes and the second-order term is obtained as

$$F_2 = \sum_n \sum_m J_{nm} \vec{S}_n \cdot \vec{S}_m, \quad (2)$$

$$J_{nm} = I^2 N_0^{-2} T \sum_\nu \sum_k \sum_{k'} \exp[i(\vec{k} - \vec{k}') \cdot (\vec{R}_n - \vec{R}_m)] \times G(\vec{k}, i\epsilon_\nu) G(\vec{k}', i\epsilon_\nu). \quad (3)$$

Here, $G(\vec{k}, i\epsilon_\nu)$ is the conduction-electron Green's function in the paramagnetic phase with wave number \vec{k} and imaginary frequency $i\epsilon_\nu$, with $\epsilon_\nu = \pi T(2\nu + 1)$, ν being an integer, and T is the temperature in energy units. J_{nm} is the well-known Ruderman-Kittel-Kasuya-Yosida indirect exchange constant between the *n*th and *m*th spins.

Next, we consider the spin-phonon interaction. The phonon is coupled with the conduction electrons via the usual electron-phonon interaction, and the spin-phonon interaction may be obtained as the cross effect of the electron-phonon and *s-f* exchange interactions. Let us introduce the perturbation Hamiltonian,

$$H' = H_{sf} + H_{ep}, \quad (4)$$

$$H_{ep} = \sum_k \sum_\sigma iq c_q u_q a_{k+\sigma}^\dagger a_{k,\sigma}, \quad (5)$$

where the subscript σ denotes the spin state, u_q is

the Fourier amplitude of the lattice vibration due to the impressed sound with wave number \bar{q} , and c_q is the electron-phonon interaction coefficient, whose explicit form will be discussed later. The spin-phonon interaction Hamiltonian is obtained through the free-energy calculation by taking I and c_q as perturbation parameters. In the order of $I^2 c_q$, we find

$$F_2' = 2I^2 T \sum_{\nu} \sum_k \sum_p i q c_q u_q G(\bar{k}, i\epsilon_{\nu})^2 \times G(\bar{k} - \bar{p}, i\epsilon_{\nu}) \bar{S}_p \cdot \bar{S}_{-p+q}, \quad (6)$$

where we introduced the Fourier transform of spins; $\bar{S}_p = N_0^{-1} \sum_n \bar{S}_n \exp(i\bar{p} \cdot \bar{R}_n)$. In particular, when the uniform spin polarization $\langle S_0^z \rangle$ exists, the component proportional to the polarization is expressed as

$$F_2' = 2iqI^2 c_q \left[\frac{\partial N(\epsilon_F)}{\partial \epsilon_F} \right] u_q \langle S_0^z \rangle S_q^z, \quad (7)$$

where ϵ_F is the Fermi energy and $N(\epsilon_F)$ is the density of states at the Fermi level. In obtaining Eq. (7), we assumed that c_q is a constant and q is negligible compared with the Fermi wave number p_F . As shown in the Appendix, the spin-phonon interaction given in Ref. 4 is expressed as

$$\sum_m (R_{n\zeta} - R_{m\zeta}) \left(\frac{\partial J_{nm}}{\partial R_{n\zeta}} \right) \exp[i\bar{p} \cdot (\bar{R}_m - \bar{R}_n)] = 2I^2 N_0^{-1} T \sum_{\nu} \sum_k c_q G(\bar{k}, i\epsilon_{\nu})^2 G(\bar{k} - \bar{p}, i\epsilon_{\nu}), \quad (8)$$

where ζ denotes the sound-propagation direction. Inserting Eq. (8) into Eq. (6), we find that the interaction (6) is just the same as the spin-phonon interaction due to the exchange modulation mechanism.^{1,2,4} We are now familiar with how to calculate the attenuation of sounds due to spins once we have the spin-phonon interaction.^{2,4,5} Therefore, the comparison between Vigren's mechanism⁷ and ours will be made in connection with the interaction Eq. (7).

In Ref. 5, the exchange striction has been derived through the calculation of the critical attenuation of sounds at the magnetic-phase-transition points. It is worthwhile to add the following on the results given in Ref. 5. By using the Thomas-Fermi approximation, the electron-phonon interaction coefficient is obtained as

$$c_q = \frac{2}{3} \epsilon_F. \quad (9)$$

If we use the coefficient, we find the attenuation calculated from the electronic density-density correlation functions, neglecting the electronic-stress-tensor terms; the stress tensor originates from the dynamical consideration of the electron-phonon interaction.^{5,6} When we use the form,

$$c_q = \frac{2}{3} \epsilon_F - \frac{k_{\zeta}^2}{m}, \quad (10)$$

in Eqs. (6) and (8), we find the result for the exchange striction given in Ref. 5. Here, k_{ζ} is the component of the electronic momentum parallel to the phonon propagation direction and m is the effective mass of the electron. In itinerant magnets, the dynamical consideration of the electron-phonon interaction is essential. The details are given in Refs. 5, 6, and 8.

The spin-phonon interaction which comes from Vigren's mechanism⁷ is as follows. The densities of the conduction electrons with up and down spins induced by the local $4f$ spins with wave number \bar{q} , \bar{S}_q^z , are expressed as

$$\delta n_1(\bar{q}) = N_1(\epsilon_F) IS_q^z, \quad (11)$$

$$\delta n_1(\bar{q}) = -N_1(\epsilon_F) IS_q^z, \quad (12)$$

where $N_{\sigma}(\epsilon_F)$ is the density of states of the σ -spin subband at the Fermi level. The electronic density fluctuation ρ_q induced by S_q^z through the s - f interaction is the sum of Eqs. (11) and (12),

$$\rho_q = \delta n_1(\bar{q}) + \delta n_1(\bar{q}) = [N_1(\epsilon_F) - N_1(\epsilon_F)] IS_q^z. \quad (13)$$

Since the phonon with wave number \bar{q} couples the electronic density with \bar{q} as $iqc_q u_q \rho_q$, we find the effective spin-phonon interaction

$$H_{sp} = iqc_q u_q [N_1(\epsilon_F) - N_1(\epsilon_F)] IS_q^z. \quad (14)$$

The densities of states in Eq. (14) are calculated to order of I as

$$N_1(\epsilon_F) - N_1(\epsilon_F) = 2 \left[\frac{\partial N(\epsilon_F)}{\partial \epsilon_F} \right] I \langle S_0^z \rangle. \quad (15)$$

Inserting Eq. (15), we have

$$H_{sp} = 2iqI^2 c_q \left[\frac{\partial N(\epsilon_F)}{\partial \epsilon_F} \right] u_q \langle S_0^z \rangle S_q^z. \quad (16)$$

Since Eq. (16) is equal to Eq. (7), it is seen that Vigren's mechanism is the same as ours. If Eq. (9) is taken as c_q , calculation using Eq. (16) gives the expression for the attenuation coefficient, Eq. (3) in Vigren's paper.⁷ We note that the exchange striction due to the uniform spin polarization is not proportional to $N(\epsilon_F)$ as mentioned in Ref. 7, but proportional to $\partial N(\epsilon_F)/\partial \epsilon_F$, if c_q is taken as a constant as seen in Eqs. (7) and (8).

In this paper, we discussed only the case of longitudinal sound. The case of transverse sounds is given in Refs. 6 and 8.

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APPENDIX: DERIVATION OF EQ. (8)

The left-hand side of Eq. (8) is rewritten using the longitudinal strain $e_{\zeta\zeta}$, as done in Ref. 2,

$$\sum_m (R_{n\zeta} - R_{m\zeta}) \left(\frac{\partial J_{nm}}{\partial R_{n\zeta}} \right) \exp[i\bar{p} \cdot (\bar{R}_m - \bar{R}_n)] = \sum_m \left(\frac{\partial J_{nm}}{\partial e_{\zeta\zeta}} \right) \exp[i\bar{p} \cdot (\bar{R}_m - \bar{R}_n)] \quad (\text{A1})$$

Inserting Eq. (3) into the right-hand side of Eq. (A1) and neglecting the spatial variation of $e_{\zeta\zeta}$, we have

$$\begin{aligned} \sum_m (R_{n\zeta} - R_{m\zeta}) \left(\frac{\partial J_{nm}}{\partial R_{n\zeta}} \right) \exp[i\bar{p} \cdot (\bar{R}_m - \bar{R}_n)] &= I^2 N_0^{-1} T \sum_\nu \left(\frac{\partial [G(\bar{k}, i\epsilon_\nu) G(\bar{k} - \bar{p}, i\epsilon_\nu)]}{\partial e_{\zeta\zeta}} \right) \\ &= I^2 N_0^{-1} T \sum_\nu \sum_k \left[\left(\frac{\partial \epsilon_k}{\partial e_{\zeta\zeta}} \right) \left(\frac{\partial G(\bar{k}, i\epsilon_\nu)}{\partial \epsilon_k} \right) G(\bar{k} - \bar{p}, i\epsilon_\nu) \right. \\ &\quad \left. + \left(\frac{\partial \epsilon_{k-p}}{\partial e_{\zeta\zeta}} \right) G(\bar{k}, i\epsilon_\nu) \left(\frac{\partial G(\bar{k} - \bar{p}, i\epsilon_\nu)}{\partial \epsilon_{k-p}} \right) \right] \\ &= 2I^2 N_0^{-1} T \sum_\nu \left(\frac{\partial \epsilon_k}{\partial e_{\zeta\zeta}} \right) G(\bar{k}, i\epsilon_\nu)^2 G(\bar{k} - \bar{p}, i\epsilon_\nu) \quad (\text{A2}) \end{aligned}$$

where ϵ_k is the energy of the electron with momentum \bar{k} . Since the derivative of ϵ_k with respect to the strain is the electron-phonon interaction coefficient⁹ introduced in Eq. (5);

$$\frac{\partial \epsilon_k}{\partial e_{\zeta\zeta}} = c_q \quad (\text{A3})$$

we find the right-hand side of Eq. (8).

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