Comment on the Deformation Potential in Ultrasonic Attenuation*

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It is pointed out that Kleinman's free-electron deformation-potential approximation is not equivalent to the method used by Pippard in calculating ultrasonic attenuation in metals. The methods are compared in terms of free-electron and band-structure contributions to the deformation energy.

A FREE-ELECTRON deformation potential (FED) approximation was used by Kleinman[1] in calculating the ultrasonic attenuation for metals having certain model Fermi surfaces. In his paper, he stated that this approximation is equivalent to the method used by Pippard[2] in deriving general expressions for the attenuation. The purpose of this paper is to point out that Pippard did not employ this approximation, and that Pippard's method is consistent with the correct formulation of the deformation potential outlined by Kleinman in an appendix.

In order to clarify the sometimes confusing terminology used by the different authors, a schematic representation of an energy band for conduction electrons is presented in Fig. 1 with important features labeled. $E(\mathbf{k})$ is the band energy in the unstrained metal, while $E'(\mathbf{k})$ is the band energy in the strained metal. In general, one expects $E'(\mathbf{k})$ to be different from $E(\mathbf{k})$ because of the changes in relative position of the ions as well as the change in density resulting from an arbitrary strain ϵ_{ij}. In the strained metal, the Fermi energy E_F' for the equilibrium electron distribution may be different from the Fermi energy E_F in the unstrained metal, consequently the Fermi wave vector $\mathbf{k}_F$ may change by $\Delta\mathbf{k}_F$, which varies with crystal direction.

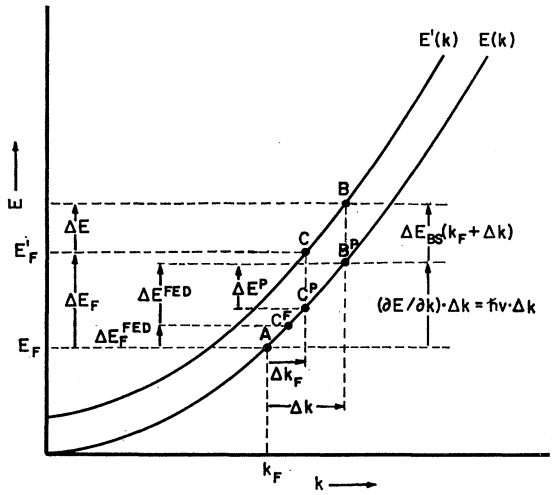

FIG. 1. Schematic representation of an energy band in a metal.

Consider an electron initially on the Fermi surface in the unstrained metal (point A). Pippard showed that a sudden strain (i.e., one which takes place in a time short compared with the relaxation time τ) shifts the electron wave vector by $\Delta k_i = -\epsilon_{ij}k_j$. He called this an adiabatic change in k because the electron is not in thermal equilibrium with the lattice. The electron ends up at B in Fig. 1, with its energy increased by $(\partial E/\partial\mathbf{k})\cdot\Delta\mathbf{k}+\Delta E_{BS}(\mathbf{k}_F+\Delta\mathbf{k})$. The first term is what Kleinman called the free-electron deformation term. It is the result of viewing the electron from a strained reference frame. The second results from the shift in the energy band when the lattice is strained.

After a time τ, the electron at B relaxes back to the equilibrium distribution at C with energy E_F'; thus the excitation energy is

$$\Delta E=\frac{\partial E}{\partial\mathbf{k}}\cdot\Delta\mathbf{k}+\Delta E_{BS}(\mathbf{k}_F+\Delta\mathbf{k})-\Delta E_F, \tag{1}$$

where

$$\Delta E_F=\left\langle\frac{\partial E}{\partial\mathbf{k}}\cdot\Delta\mathbf{k}\right\rangle_{\mathrm{FS}}+\langle\Delta E_{BS}\rangle_{\mathrm{FS}}, \tag{2}$$

and $\langle\ \rangle_{\mathrm{FS}}$ indicates an average over the Fermi surface. However, one can also describe the Fermi energy shift in terms of $\Delta\mathbf{k}_F$, the shift in Fermi wave vector normal to the Fermi surface:

$$\Delta E_F=\frac{\partial E}{\partial\mathbf{k}}\cdot\Delta\mathbf{k}_F+\Delta E_{BS}(\mathbf{k}_F+\Delta\mathbf{k}_F), \tag{3}$$

so that

$$\Delta E=\frac{\partial E}{\partial\mathbf{k}}\cdot(\Delta\mathbf{k}-\Delta\mathbf{k}_F), \tag{4}$$

since

$$\Delta E_{BS}(\mathbf{k}_F+\Delta\mathbf{k})=\Delta E_{BS}(\mathbf{k}_F+\Delta\mathbf{k}_F)$$

to first order. Pippard computes the excitation energy from

$$\Delta E^P=\hbar\mathbf{v}\cdot(\Delta\mathbf{k}-\Delta\mathbf{k}_F), \tag{5}$$

which is identical with Eq. (4) to this order. Note that ΔE^P is just the difference in energies at B^P and C^P in Fig. 1, which might lead one to believe that changes in the energy band caused by strain have been ignored.

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[1] Leonard Kleinman, Phys. Rev. **182**, 686 (1969).
[2] A. B. Pippard, Proc. Roy. Soc. (London) **A257**, 165 (1960).

However, all such effects are included in Pippard's fitting parameter K_{ij}, where

$$\Delta\mathbf{k}_F = \mathbf{n}\epsilon_{ij}K_{ij}(\mathbf{k}_F), \tag{6}$$

and $\mathbf{n}$ is a unit vector perpendicular to the Fermi surface. One could calculate K_{ij} from first principles along the lines suggested by Kleinman in his appendix, or one might measure it with the de Haas–van Alphen effect in crystals with known strains.

Kleinman has suggested a model for studying deformation-potential effects when the actual deformation potential is not known. He makes use of parameters which may be available from experiments or ordinary band calculations, $\mathbf{k}_F$ and $\mathbf{v}_F$, and retains only the first term on the right-hand side of Eq. (1). With Pippard, he considers the excited electron to be at B^P with energy $(\partial E/\partial\mathbf{k})\cdot\Delta\mathbf{k}$. However, instead of treating the Fermi-surface shift as an unknown parameter, he computes it from Eq. (2). Since the second term vanishes for the FED model, he finds

$$\Delta E_F{}^{\mathrm{FED}} = \langle(\partial E/\partial\mathbf{k})\cdot\Delta\mathbf{k}\rangle_{\mathrm{FS}}, \tag{7}$$

indicated by C^F in Fig. 1.

Using (1), (2), and (7) we find that the error which results from the FED approximation is

$$\Delta E - \Delta E^{\mathrm{FED}} = \Delta E_{BS}(\mathbf{k}_F) - \langle\Delta E_{BS}\rangle_{\mathrm{FS}}. \tag{8}$$

In this case of metals for which $\mathbf{k}_F$ and $\mathbf{v}_F$ are known, one could study discrepancies between measured attenuation and that calculated using the FED model to learn the relative importance of the error described by Eq. (8) for the electrons which dominate the attenuation.

I should like to express my appreciation to Professor A. B. Pippard and to Professor L. Kleinman for helpful discussions of their respective papers.

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Interpretation of the Mössbauer Isomer Shift in ^{119}Sn†

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The determination by the internal-conversion method of the fractional charge-radius change $\delta R/R$ for the 23.9-keV $M1$ transition in ^{119}Sn is reexamined. A modified $\delta R/R$ value is obtained; this is compared with values otherwise determined, and some implications of these comparisons are derived.

IN a letter[1] on chemical effects on valence-electron internal conversion of the 23.9-keV magnetic dipole transition in ^{119}Sn, and on interpretation of the Mössbauer isomer shift for that transition, it was reported that the ratio of O-shell-to-N_1-shell conversion is (0.108 ± 0.004) when the source is in the form of white tin metal and (0.074 ± 0.004) when in the form SnO_2. The derivation from these experimental results of the change in charge radius of ^{119}Sn upon excitation needs modifications which produce effects on the magnitude of $\delta R/R$ but not on its sign. After rederiving the result for $\delta R/R$, we comment on the results implied for the internal-conversion experiment by other interpretations of the isomer shift.

First, an error was made in Ref. 1 in the values of s electron density at the nucleus.[2] From the results of the Hartree-Fock-Slater calculations of Herman and Skillman,[3] we find the nonrelativistic electron density at the nucleus for the two $4s$ electrons to be

$$|\Psi_{4s}(0)|^2 = 320.8a_0^{-3}.$$

The experimental results[1] then imply that between β-Sn and SnO_2 the change in valence electron density (equivalent nonrelativistic density) at the nucleus is

$$(|\psi_{5s}(0)|_{\beta\text{-Sn}}{}^2 - |\psi_{5s}(0)|_{SnO_2}{}^2) = (10.9\pm1.8)a_0^{-3},$$

where the uncertainty shown is due to the experimental uncertainty and does not include any contribution from

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[1] J.-P. Bocquet, Y. Y. Chu, O. C. Kistner, M. L. Perlman, and G. T. Emery, Phys. Rev. Letters **17**, 809 (1966).

[2] For which the present authors were responsible. We wish to thank Dr. F. Pleiter and Dr. Hans Postma for calling to our attention the possibility of such an error.
[3] F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, N. J., 1963).