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Eliashberg function in amorphous metals

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An expression for the Eliashberg function $\alpha^2F(\omega)$ is derived for amorphous metals beginning with a formulation in terms of the Van Hove dynamical structure factor. The result is equivalent to one derived from a different starting point by Poon and Geballe. At low energy, $\alpha^2F(\omega)$ is shown to vary linearly with ω and inversely with the electron mean free path Λ in agreement with Bergmann's expression derived for a Gaussian-disordered crystalline metal. Modification of the theory for short mean free paths is discussed in terms of the Pippard-Ziman condition on the electron-phonon interaction. Invoking a prescription derived by Pippard for the reduction of the electron-phonon interaction in ultrasonic attentuation, one finds a quadratic dependence of $\alpha^2F(\omega)$ on ω at low energies in high-resistivity amorphous metals; an even sharper reduction in the electron-phonon interaction and hence in $\alpha^2F(\omega)$ has been found by Poon, who treated the problem in transition-metal systems in the context of the Barisic-Labbe-Friedel rigid-ion approximation.

I. INTRODUCTION

The Van Hove dynamical structure factor[1] $S(K,\omega)$ plays an important role in the description of the lattice-dynamical properties of metals. Baym[2] has given explicit expressions for the electron self-energy, mass-enhancement factor, and the electrical and thermal conductivity in terms of only the effective electron-lattice matrix element and $S(K,\omega)$. Meisel and Cote[3] have given expressions for $S(K,\omega)$ appropriate for amorphous metals. Baym's equations lead to the Ziman-Faber theory of liquid-metal electrical transport[4] and the corresponding result for amorphous-metal electrical transport.[5] The Eliashberg function[6] $\alpha^2F(\omega)$ is an electron-phonon interaction-weighted density of states and is central to the theory of superconductivity. In this paper we derive an expression for $\alpha^2F(\omega)$ appropriate for amorphous metals beginning with a formulation in terms of $S(K,\omega)$ as proposed by Baym[2]; the result is given in terms of the phonon-branch densities of states and dispersion relations, the effective electron-lattice matrix elements (t matrices), and the geometrical structure factor. Our result is seen to be equivalent to one derived by Poon and Geballe[7] who started from an expression for $\alpha^2F(\omega)$ given by Allen.[8]

The connection between the Ziman-Faber liquid-metal theory[4,5] resistivity and the Eliashberg function (as reported by Poon and Geballe[7] and by Bergmann[9]) is clearly seen in the unified treatment in terms of the Van Hove dynamical structure factor. In particular, it is shown that $\alpha^2F(\omega)$ for small ω is inversely proportional to the electron mean free path Λ. It is remarkable that such a relationship exists despite the fact that elastic scattering processes play the dominant role in determining the magnitude of Λ in the amorphous or liquid state while inelastic (electron-phonon) scattering determines $\alpha^2F(\omega)$.

The form of $\alpha^2F(\omega)$ for the dominant backscattering case, which is expected to be relevant to transition-metal-based alloys, is also presented. A modification of the theory, based upon the Pippard-Ziman condition on the electron-phonon interaction,[10,11] is suggested for high-resistivity (short Λ) metals (for which weak scattering theory is expected to fail). The results of this approach are compared with recent calculations of Poon[12] in which the reduced electron-phonon interaction in disordered alloys is computed within the Barisic-Labbe-Friedel rigid-atom approximation.[13]

II. THEORY

A. Van Hove dynamical structure factor

The Sham-Ziman form of the dynamical structure factor appropriate to amorphous metals[3,14] is given by

$$S(K,\omega)=S_0(K,\omega)+S_{\rm ph}(K,\omega)\quad , \tag{1}$$

where the elastic part

$$S_0(K,\omega)=e^{-2W(K)}a(K)\delta(\omega)\quad , \tag{2}$$

with $e^{-2W(K)}$ the Debye-Waller factor and $a(K)$ the geometrical structure factor. The phonon part

$$S_{\rm ph}(K,\omega)=\sum_\alpha S_\alpha(K,\omega)\quad , \tag{3a}$$

where the sum runs over the branches of the phonon spectrum and the α branch contribution is given by

$$\begin{aligned} S_\alpha(K,\omega) &= [n(\omega)+1] \sum_{q_\alpha} \frac{\hbar K^2/3}{2M\omega} [a(\bar{K}-\bar{q}_\alpha)\delta(\omega-\omega_{q_\alpha})+a(\bar{K}+\bar{q}_\alpha)\delta(\omega+\omega_{q_\alpha})] \\ &\equiv \hbar K^2[n(\omega)+1]\sigma_\alpha(K,\omega)/6M\omega \ , \end{aligned} \tag{3b}$$

where $\hbar$ is Planck's constant over 2π, $n(\omega)$ is the phonon occupation number, M is the ionic mass, the sum runs over the α branch of the phonon spectrum, and we have used the isotropy of the amorphous state. Converting the sum into an integral over the phonon spectrum, we have

$$\sigma_\alpha(K,\omega) = \int_0^\infty d\omega_{q_\alpha} F_\alpha(\omega_{q_\alpha}) \int \frac{d\Omega\, q_\alpha}{4\pi} [a(\bar{K}-\bar{q}_\alpha)\delta(\omega-\omega_{q_\alpha})+a(\bar{K}+\bar{q}_\alpha)\delta(\omega+\omega_{q_\alpha})]$$

$$= F_\alpha(|\omega|) \int \frac{d\Omega\, q_\alpha}{4\pi} a(\bar{K}-\bar{q}_\alpha(\omega)) \tag{4a}$$

$$\equiv F_\alpha(|\omega|) A(K,q_\alpha(\omega)) \ , \tag{4b}$$

where $F_\alpha(\omega)$ is the α branch phonon density of states, $q_\alpha(\omega)$ is the α branch dispersion relation, and we have defined a q-dependent averaged structure factor $A(K,q)$.

Combining terms for the longitudinal (l), two transverse (t) acoustic branches, and the optical branches one obtains

$$\begin{aligned} \sigma(K,\omega) &= \sum_\alpha \sigma_\alpha(K,\omega) \\ &= F_l(\omega)A(K,q_l(\omega)) + 2F_t(\omega)A(K,q_t(\omega)) \\ &\quad + \sum_i F_{0i}(\omega)A(K,q_{0i}(\omega)) \ , \end{aligned} \tag{5}$$

where the sum on i runs over the optical branches.

B. Transport relaxation time τ_e

The dominant contribution to the electrical resistivity of amorphous metals is produced by elastic scattering and at low temperatures the Debye-Waller factor is approximately unity. Thus,[5,15] with $x \equiv \hbar\omega/k_BT$,

$$\frac{1}{4\pi\tau_e} = C\int_{-\infty}^{\infty} d\omega \int_0^1 d\left(\frac{K}{2k_F}\right)\left(\frac{K}{2k_F}\right)^3 \times xn(x)S(K,\omega)|t(K)|^2 \tag{6}$$

$$\approx C\int_0^1 d\left(\frac{K}{2k_F}\right)\left(\frac{K}{2k_F}\right)^3 a(K)|t(K)|^2 \ , \tag{7}$$

where k_B is Boltzmann's constant, T is the temperature, k_F the Fermi wave number, $t(K)$ the scattering matrix, and $C \equiv 3Z/2\hbar E_F$ with Z the effective valence and E_F the Fermi energy. Equation (6) is equivalent to the expression given by Baym.[2]

If backscattering is dominant

$$\frac{1}{4\pi\tau_e} \approx \frac{C}{4} a(2k_F)|t(2k_F)|^2 \ . \tag{8}$$

We shall also use the following definition of the electron mean free path Λ:

$$\Lambda \equiv V_F\tau_e = \hbar k_F\tau_e/m \ , \tag{9}$$

where V_F is the Fermi velocity and m the electron mass.

C. Mass-enhancement factor λ and Eliashberg function $\alpha^2F(\omega)$

The mass-enhancement factor is given by

$$\lambda \equiv 2\int_0^\infty \frac{d\omega}{\omega}\alpha^2F(\omega) \tag{10}$$

$$= 2\int_{-\infty}^{\infty} \frac{d\omega}{\omega} C \int_0^1 d\left(\frac{K}{2k_F}\right)\left(\frac{K}{2k_F}\right) S(K,\omega)|t(K)|^2 \ , \tag{11}$$

where the usual definition of the Eliashberg function[6] is contained in Eq. (10) and Eq. (11) is equivalent to the expression given by Baym.[2] Thus,

$$\alpha^2F(\omega) = \frac{2\hbar k_F^2}{3M\omega} C\int_0^1 d\left(\frac{K}{2k_F}\right)\left(\frac{K}{2k_F}\right)^3 \times |t(K)|^2\sigma(K,\omega) \ , \tag{12}$$

where we have used the identity

$$\int_{-\infty}^{\infty} d\omega\, \omega^{-2} n(\omega)G(|\omega|) \equiv -\int_0^\infty d\omega\, \omega^{-2}G(\omega) \ ,$$

and $\sigma(K,\omega)$ is defined in Eq. (5). The form of Eqs. (5) and (12) indicates that α^2F does not factor in the general case. Equation (12) is equivalent to the expression derived by Poon and Geballe[7] who began from an equation given by Allen.[8] We now consider some special cases.

i. Small energy (low ω) limit. In this limit there are no optical modes and both $q_t(\omega)$ and $q_l(\omega)$ are small. Thus

$$A(K,q_\alpha(\omega)) \to a(K), \quad \alpha = l,t \tag{13a}$$

and

$$F_\alpha(\omega) \to \frac{3\omega^2}{(q_D c_\alpha)^3}, \quad \alpha = l,t \ , \tag{13b}$$

where q_D is the wave number and c_α is the α branch sound velocity. Thus,

$$\alpha^2F(\omega) \to \frac{2\hbar k_F^2}{3M\omega} C \int_0^1 d\left(\frac{K}{2k_F}\right)\left(\frac{K}{2k_F}\right)^3 |t(K)|^2 \times a(K)\frac{3\omega^2}{q_D^3}\left(\frac{1}{c_l^3}+\frac{2}{c_t^3}\right)$$

$$= \left(\frac{2\hbar k_F^2}{3M\omega}\frac{1}{4\pi\tau_e}\right)F(\omega) \tag{14a}$$

$$= \frac{2\hbar}{4\pi Mm}\left(\frac{1}{c_l^3}+\frac{2}{c_t^3}\right)\frac{\hbar\omega}{\Lambda} \ , \tag{14b}$$

where we have used Eqs. (7) and (9) and the free-electron identity $2k_F^3 \equiv Zq_D^3$. $\alpha^2F(\omega)$ factors into $\alpha^2(\omega)F(\omega)$ as displayed in Eq. (14a). Equation (14b) is identical to that derived for the small ω limit of a "Gaussian-disordered" crystalline metal by Bergmann.[9]

The low-energy limiting form of the Eliashberg function is especially important because of the extra weight given to low energies in the expression for the mass-enhancement factor.

ii. Backscattering dominant. When backscattering is dominant, Eq. (12) can be brought to the form,

$$\alpha^2F(\omega) \cong \frac{\hbar k_F^2}{6M\omega} C\sigma(2k_F,\omega)|t(2k_F)|^2$$

$$= \frac{2\hbar k_F^2}{3M\omega}\frac{1}{4\pi\tau_e}\frac{\sigma(2k_F,\omega)}{a(2k_F)}$$

$$= \frac{Z\hbar}{4\pi mM}\frac{q_D^3}{3\omega^2}\frac{\sigma(2k_F,\omega)}{a(2k_F)}\frac{\hbar\omega}{\Lambda} \ . \tag{15}$$

iii. Backscattering dominant and a $(2k_F)$ near unity. When $a(2k_F)$ is near unity, the averaged structure factors $A(2k_F,q)$ become essentially q independent and approximately equal to $a(2k_F)$; thus

$$\sigma(2k_F,\omega) \cong a(2k_F)F(\omega) \tag{16}$$

and Eq. (15) assumes the form

$$\alpha^2F(\omega) = (Z\hbar^2 q_D^3/12\pi mM\omega\Lambda)F(\omega) \ . \tag{17}$$

D. Pippard-Ziman condition

We have suggested in earlier work[16] that the electron-phonon interaction should be modified in high-resistivity metals in accord with the condition (as stated by Ziman[10]), "Phonons whose wavelengths $2\pi/q$ exceed the electron mean free path Λ are ineffective electron scatterers." Pippard's work[11] contains an analytic expression, the Pippard function $P(q\Lambda)$, for the reduction of the electron-phonon interaction which results at small Λ. These ideas are established in the theories of ultrasonic attenuation[17] and thermal conductivity[18] of high-resistivity metals; but their applicability to electrical transport[16] and superconductivity[16] is still open to question.

The Pippard function is given as

$$P(x) = (2/\pi)[x\tan^{-1}x/(x-\tan^{-1}x) - 3/x] \ . \tag{18a}$$

Useful approximate forms at large and small x are

$$P(x) \cong 8x/5\pi, \quad x < 1.5 \tag{18b}$$

and

$$P(x) \cong 1 - 0.976/x, \quad x > 5 \ . \tag{18c}$$

If the Pippard-Ziman condition describes the reduction in the electron-phonon interaction at small $q\Lambda$, then the previously given formulas should be amended according to the prescription;

$$\alpha^2F(\omega)_p = \alpha^2F(\omega)P(q(\omega)\Lambda) \ . \tag{19}$$

In particular, this implies that in high-resistivity metals the low-energy form of α^2F would be given by

$$\alpha^2F(\omega)_p \approx \frac{2}{5\pi^2 Mm}\left(\frac{1}{c_l^2}+\frac{2}{c_t^4}\right)(\hbar\omega)^2 \tag{20}$$

for $q(\omega)\Lambda$ less than about 2. That is, in high-resistivity amorphous metals, the low-energy part $[q(\omega)\Lambda \leqslant 2]$ of the Eliashberg function will be quadratic as is usually found in crystalline metals.

Recently Poon[12] has computed a reduction in electron-phonon interaction (which he refers to as "phonon ineffectiveness"), based upon the Barisic-Labbe-Friedel rigid-ion approximation[13] appropriate for systems where localization is becoming important. He finds α^2F proportional to ω^3 at small ω in high-resistivity systems and a much greater reduction than is given by the prescription of Eq. (19). This can be taken as further theoretical justification for imposing the Pippard-Ziman condition in the treatment of strong scattering systems; it also suggests that the Pippard function underestimates the reduction of the electron-phonon interaction in such systems.

III. DISCUSSION

It is shown that a consistent approach, as outlined by Baym,[2] can be applied, in particular, to electrical transport and the Eliashberg function in amorphous metals. The application to electrical transport gives rise to the Ziman-Faber theory[4,5] as is well known. The application to the Eliashberg theory as given here gives results equivalent to those derived by Poon and Geballe[7] based upon an equation of Allen.[8] The expression in Eq. (12), for $q\Lambda$ not too small, gives $\alpha^2F(\omega)$ in terms of the branch phonon densities of states $F_\alpha(\omega)$ and dispersion relations $q_\alpha(\omega)$, geometrical structure factors $a(K)$, and the scattering t matrix $t(K)$. Equation (14) indicates that the small energy behavior of α^2F is linear in ω and inversely proportional to Λ. If backscattering is dominant (as might be the case in transition-metal-based systems) Eq. (15) shows that α^2F will be inversely proportional to Λ and will be determined by averages of the geometrical structure factor near $2k_F$ as well as the phonon-branch densities of states and dispersion relations. If backscattering is dominant and $a(2k_F)\approx 1$, Eq. (17) shows that α^2F is approximately proportional to $F(\omega)/\omega\Lambda$.

The small-ω behavior of α^2F is important because of the extra weight given to low-energy modes in the expression for the mass-enhancement factor λ and is given by Eq. (14) which is equivalent to Bergmann's result[9] derived for a simple model of a disordered crystalline metal. As pointed out by Bergmann[9] α^2F is enhanced at small ω in amorphous metals as compared to crystalline metals because (i) α^2F is linear rather than quadratic in ω, (ii) there is a large increase in $F(\omega)$ associated with a decrease in c_t found in disordered systems (which is also responsible for a large increase in the T^3 part of the specific heat), and (iii) the electron mean free path Λ tends to be shorter in amorphous alloys.

The enhanced values of α^2F relative to crystalline alloys in the important small-ω regime lead one to expect that amorphous alloys will be better superconductors than their crystalline counterparts. This expectation is apparently realized in amorphous simple metal systems,[19] which, as Bergmann emphasized,[9] behave like strong coupled superconductors. However, amorphous transition-metal systems do not fit the pattern. Collver and Hammond[20] demonstrated that in amorphous transition-metal alloys, T_c varies smoothly with the electron-per-atom ratio, exhibiting a broad maximum near 6.5 in contrast to the double-peaked variation seen in crystalline transition metals,[21] and T_c in the amorphous phase of the highest T_c crystalline alloys is only about half as large. This variation of T_c in amorphous transition metals remains to be explained.

The most striking aspects of Eq. (14) [Bergmann's Eq. (5.6)] is that α^2F should be linear in ω at small ω. This prediction has been confirmed in many amorphous and disordered alloys.[22] However, for small Λ (corresponding to resistivities in excess of 100 $\mu\Omega$ cm) the Pippard-Ziman condition[10,11] may become important. Cote and Meisel[16] used a sharp cutoff in the electron-phonon interaction at small ω to approximate the effect of the Pippard-Ziman condition and found that this could explain the degradation of T_c seen in some radiation-damaged superconductors[23] and "saturation effects" in the electrical resistivity of high-resistivity metals.[24] A Pippard function modification as in Eq. (19) is probably a more realistic approach because it correctly describes the $q\Lambda$ dependence of the ultrasonic attenuation,[17] "saturation effects" in electrical resistivity,[5] and the thermal conductivity of high-resistivity metals[18]; however, it yields a quadratic small-ω form for $\alpha^2F(\omega)$ [Eq. (20)] which is *not* reduced sharply enough to explain the observed degradation of T_c in radiation-damaged superconductors. Poon's calculations,[12] within the Barisic-Labbe-Friedel approximation,[13] yield a more sharply reduced low energy $\alpha^2F(\omega)$, proportional to ω^3, in systems where electron localization is becoming important and thus may be more successful in explaining the degradation in T_c.

Recent measurements[25] of α^2F in high-resistivity amorphous metals exhibit curvature at small ω in accord with the results of the Pippard-Ziman condition which suggests that this is a fruitful approach. Obviously, serious questions remain concerning the nature of the reduction of the electron-phonon interaction in high-resistivity amorphous metals; detailed tunneling experiments in high-resistivity amorphous alloys would be helpful in this regard.

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