Assessment of theoretical determinations of the electron-phonon coupling parameter λ in metals and intermetallic compounds

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The electron-phonon coupling parameter $\lambda_{e\text{-ph}}$, while playing a centrally important role in superconductivity and other phenomena, is still a difficult quantity to determine from first-principles theory. The availability of accurate *ab initio* self-consistent energy-band calculations of partial and total density of states (DOS) allows λ to be determined from the electronic specific heat or from simple theoretical treatments such as the rigid-ion approximation. We have assessed the accuracy of these determinations (and the band-structure results) in a number of transition metals and $A15$ and $C15$ intermetallic compounds. We include comparisons with results obtained with the use of the McMillan-equation parametrization of T_c along with experimental results from tunneling measurements, NMR, and comparisons of high- and low-T specific-heat data. The results of these comparisons show that for many of the high-DOS materials, serious discrepancies exist between the theoretical and experimental determinations. The role of spin fluctuations and lattice transformations is discussed in connection with these results.

I. INTRODUCTION

The electron-phonon parameter $\lambda_{e\text{-ph}}$ is a quantity of prime importance to superconductivity and other phenomena; at the same time its accurate determination from experiment or first-principles theory is often difficult. The availability of accurate energy-band calculations of the electronic density of states (DOS) in conjunction with the electronic heat capacity allows $\lambda = \lambda_{e\text{-ph}} + \lambda_{\text{spin}}$ to be calculated for many important systems, including the transition-metal elements and $A15$, and $C15$ compounds. The total enhancement of the heat capacity[1] can be written as

$$\gamma = \tfrac{1}{3}\pi^2 k_B^2 N(E_F)(1+\lambda_{e\text{-ph}}+\lambda_{\text{spin}}) = \frac{m^*}{m}\gamma_0 ,$$

(1)

where $N(E_F)$ is the bare DOS which would result

from an exact band-structure calculation,[2-14] and γ_0 is the enhanced value of the electronic heat-capacity coefficient. The terms involving $\lambda_{e\text{-ph}}$ and λ_{spin} express the mass enhancement which arises due to the electron-electron exchange interactions, in the first case mediated by phonons, while in the second by dynamic spin fluctuations.[1] The value of $\lambda_{e\text{-ph}}$ can also be calculated from simple treatments such as the rigid-ion approximation.[15] In this paper the convention has been adopted that λ denotes the total mass enhancement, $m^*/m = 1+\lambda$. When only the electron-phonon enhancement is considered, it is written as $1+\lambda_{e\text{-ph}}$.

Materials such as the $A15$ and $C15$ compounds show many interesting phenomena including high-T_c superconductivity and lattice instabilities, as well as itinerant magnetism in $ZrZn_2$ and $TiBe_{1.8}Cu_{0.2}$. In these materials, band-structure

calculations have been very important in under-
standing these phenomena, particularly those relat-
ing to the electron-phonon interaction. In order to
make full use of these theoretical calculations,
however, it is necessary to have some measure of
the accuracy of the band-structure results and the
λ values which are derived from them. This type
of information accomplishes a dual purpose. First,
it allows error bars to be placed on quantities
which use $N(E_F)$ or λ as input parameters. The
experimental determination of λ from de
Haas—van Alphen (dHvA) data,[16-18] as well as re-
cent attempts to separate the spin-fluctuation con-
tribution to the heat capacity by Rietschel and
Winter[19] in Nb and V, and Orlando and Beasley[20]
in some A15 compounds are examples of this situa-
tion. Second, by critically examining the accuracy
of theoretical calculations of λ for a number of
different materials, problems which are of a gen-
eral nature can be identified. For this paper, we
have conducted a critical survey of the available
DOS calculations for some of the transition metals,
as well as the A15 and C15 compounds. Our ap-
proach has been to evaluate the accuracy of the
calculations and of the λ values derived from them
by comparison with all available experimental
values. It should be noted that some methods
determine the total mass enhancement λ, while
others give $\lambda_{e\text{-ph}}$ directly. The value of λ_{spin} is very
difficult to determine either from theory or experi-
ment, so for the purposes of comparing with exper-
iment, λ_{spin} is assumed small and so neglected. In
materials where large discrepancies are found, this
assumption will be reconsidered and the evidence
for spin fluctuation will be discussed. This review
also serves the purpose of compiling in consistent
units the results of many workers on these materi-
als.

This paper is organized as follows. Section II
outlines the different methods and approximations
used to calculate the DOS. In general, different
approximations give fairly consistent results for
most materials considered, and rough estimates of
the errors involved are discussed. Section III
discusses the experimental methods and available
data for λ. The value of $\lambda_{e\text{-ph}}$ can be determined
from tunneling experiments,[21-33] while λ can be
found using nuclear-magnetic-resonance (NMR)
measurements[34-36] in conjunction with electronic
heat-capacity determinations or from comparisons
of high- and low-temperature heat-capacity
data.[37-40] In addition, $\lambda_{e\text{-ph}}$ can be determined
from observed superconducting T_c values through

the use of the McMillan equation[41] or one of its
improved versions[42]; these values are presented as
well. Section IV compares the values of $N(E_F)$
and $\lambda_{e\text{-ph}}$ from theory and experiment; large
disagreements are found for some materials. Sec-
tion V discusses the results and draws conclusions.

II. THEORETICAL CONSIDERATIONS

A. Methods

In order to obtain accurate values of $N(E_F)$ we
consider the fairly recent local density band calcu-
lations. In these, the potential is described as a
one-electron local potential which includes the
electron-electron interaction as an electron-
density-dependent interaction. Different forms of
the local density approximation exist and are used,
but since they all give satisfactory results, their
differences are not interesting for our purposes
here. It is desired, in modern band theory, to have
both self-consistent (SC) and a general potential
(i.e., beyond the assumption of a spherically sym-
metric potential inside a constant potential in the
interstitial region) calculation. Most of the calcu-
lations we review are in fact self-consistent, but do
not always include a general potential.

Other factors, such as the number of k points in
the irreducible Brillouin zone at which the eigen-
values have been determined, affect the quality of
the results. Apparently, the number of k points
used is roughly inversely proportional to the num-
ber of atoms per unit cell, but as a standard, 89
points for one atom per cell could be considered to
be sufficient and all results quoted in this paper
use this or more first-principles points. Often, to
go beyond this level, a k-point interpolation pro-
cedure is adopted which improves the k-point sam-
pling. Thus, a Fourier-fitting procedure is com-
monly used to fit the energy bands and finally a
$\vec{k}$-space volume integration scheme such as the
tetrahedron method might be added to calculate
the DOS more precisely. All these methods can be
applied to different degrees of sophistication, but it
is hard to give a well-defined "error bar" for the
theoretically determined $N(E_F)$ for a given first-
principles energy-band calculation due to various
factors. Loosely, one would expect an accuracy of
$10-15\%$ for any DOS presented, given an energy
resolution of about 2 mRy.

The DOS at E_F is a very sensitive quantity es-
pecially for many of the materials studied here be-

cause E_F falls at either a high peak or in a region of rapid variation in the DOS. Hence when comparing to experimental systems, it should be remembered that the band structure is for a perfect crystal; in reality one may have lattice imperfections, impurity vacancies, or subtle lattice distortions, and for compounds even nonstoichiometry or multiphase systems.

For calculating the electron-phonon coupling parameter $\lambda_{e\text{-ph}}$ and superconducting transition temperature T_c, one usually relies on the applicability of the rigid-ion approximation[15] and the McMillan equation[41] for strongly coupled superconductors. Here, we generally refer to calculated results based on these approximations. However, Rietschel and Winter[19] have recently pointed out the possible importance of spin fluctuations in Nb and V and have attempted to go beyond the rigid-ion approximation. In the rigid-ion formulation, $\lambda_{e\text{-ph}}$ is separated into an "electronic" numerator and a pure "phonon"-dependent denominator,

$$\lambda_{e\text{-ph}} = \frac{\eta}{M\langle\omega^2\rangle} \ . \tag{2}$$

Here, M is the atomic mass and $\langle\omega^2\rangle$ is an average over the square of the phonon spectrum. The use of Eq. (2) is a severe approximation, especially in compounds where there are different possibilities to average over several sites, and the information about $\langle\omega^2\rangle$ is obtained experimentally, either from heat-capacity measurements or by weighting the phonon spectrum if it is known from neutron data. The matrix element η is usually determined from the rigid-muffin-tin (RMT) Gaspari-Gyorffy[15] formula,

$$\eta = \frac{\sqrt{E_F}}{\pi^2 N(E_F)} \sum_l (l+1)\sin^2(\delta_l - \delta_{l+1})$$
$$\times \frac{N_l(E_F)N_{l+1}(E_F)}{N_l^0(E_F)N_{l+1}^0(E_F)} \ , \tag{3}$$

where $N_l(E_F)$ and $N_l^0(E_F)$ are band DOS at E_F and DOS for a free scatter, respectively. The phase shifts δ_l and δ_{l+1} are determined at the surface of the "muffin-tin" sphere and the evaluation is fairly straightforward.

The T_c is determined from $\lambda_{e\text{-ph}}$ using the McMillan[41] (or the related Allen-Dynes[42]) equation,

$$T_c = \frac{\Theta_D}{1.45}\exp\left[-\frac{1.04(1+\lambda_{e\text{-ph}})}{\lambda_{e\text{-ph}} - \mu^*(1+0.62\lambda_{e\text{-ph}})}\right] , \tag{4}$$

where Θ_D is the Debye temperature in the former[41] or some mean value of the phonon spectrum in the latter case.[42] The electron-electron coupling parameter μ^* is usually taken to be 0.13 or can be calculated from the total DOS through the empirically derived formula of Bennemann and Garland,[43]

$$\mu^* = 0.26N(E_F)/[1+N(E_F)] \ . \tag{5}$$

B. The pure elements

The pure elements have been studied recently in several independent band-structure calculations which are presented in Table I. The corresponding RMT results for $\lambda_{e\text{-ph}}$ are shown in Table II. These results represent very well the present theoretical situation, and are generally in agreement to $\pm 10\%$. In general, these calculations may be considered to be fairly precise, since any neglect of nonspherical contributions to the potential is not so severe for these close-packed elements. The consistency of the results for $N(E_F)$ is shown graphically in Fig. 1. Papaconstantopoulos et al.[2] employed the self-consistent Korringa-Kohn-Rostoker (KKR) band method for several elements with $Z < 50$. The assumption was made that the structures are bcc or fcc only. Their subsequent electron-phonon coupling calculations[2] used the SC-KKR potentials as input to a one-step, muffin-tin, augmented-plane-wave (APW) calculation using $\sim 250\ k$ points and a quadratic interpolation method to obtain higher-resolution DOS values for the electron-phonon coupling calculations using the rigid-ion approximation. The averaged phonon frequency $\langle\omega^2\rangle$ was taken as $1/2\Theta_D^2$ where Θ_D is the experimental Debye temperature.

Glötzel et al.[3] have performed self-consistent linear-muffin-tin orbital (LMTO) calculations for a number of transition metals employing the atomic sphere approximations. These results then served as input to the rigid-muffin-tin approximation calculations of $\lambda_{e\text{-ph}}$. Skriver et al.[6] have calculated self-consistently the band structure for Y with the LMTO method, including some relativistic effects. Self-consistent relativistic linear-augmented-plane-wave (LAPW) calculations for La were performed by Pickett et al.[4] For Pt and Pd we quote a recent high-precision relativized LAPW result of MacDonald et al.[5] As a maximum difference for the DOS from different calculations we can take the Pd results of Papaconstantopoulos et al.[2] (2.18 eV^{-1}) and those of MacDonald et al.[5] (2.55 eV^{-1}), to obtain a difference of $\sim 17\%$.

TABLE I. Values of $N(E_F)$ for some transition-metal elements. $N(E_F)$ is in units of states/eV atom both spins and γ is in units of mJ/g atom K^2. Theoretical, experimental, and empirical values from the McMillan equation are shown. Quantities which were converted from λ values through Eq. (1) are listed as λ_γ. The values of T_c, Θ_D, and λ for these materials are also listed.

Material	T_c[a]	γ	Θ_D	Theory band-structure calculation $N(E_F)$	Experiment High-low temperature heat capacity $N(E_F)$[b]	Tunneling $N_\gamma(E_F)$	Empirical McMillan equation $N_\gamma(E_F)$
Nb	9.26	7.6[b]	280[b]	1.43[c] 1.33[b]	1.66±0.1	1.58[d]	1.695
La(fcc)	6.05	11.5[f]	140[f]	2.02[g]			2.344
V	5.38	8.8[b]	378[b]	1.81[a] 1.79[e]	1.82±0.16	2.08[h]	2.182
Ta	4.48	5.8[b]	222[b]	1.18[e]	1.23±0.3	1.45[i] 1.46[j]	1.423
Mo	0.92	2.0[f]	470[f]	0.65[c] 0.57[e]			0.624
Pd	<0.01	9.2[b]	275[b]	2.18[c] 2.47[e] 2.55[k]	2.28±0.16		>2.832
Pt	<0.01	6.7[b]	229[b]	2.06[b] 1.8[k]	1.7 ±0.08		>2.095
Sc	<0.01	10.7[b]	313[b]	2.31[c]	3.31±0.12		>3.273
Y	<0.03	10.1[b]	214[b]	1.61[c] 1.83[l]	3.23±0.12		>3.030

[a]See Ref. 1.
[b]See Ref. 38.
[c]See Ref. 2.
[d]See Ref. 24.
[e]See Ref. 3.
[f]See Ref. 60.

[g]See Ref. 4.
[h]See Ref. 26.
[i]See Ref. 22.
[j]See Ref. 27.
[k]See Ref. 5.
[l]See Ref. 6.

C. A15 compounds

For the A15 compounds we use results from the five independent energy-band studies shown in Table III. From Fig. 1 it is clear that the calculations are consistent for most of the compounds with the exception of Nb$_3$Sn and Nb$_3$Ge which show a substantial variation. Mattheiss et al.[9] have used a non-self-consistent augmented-plane-wave linear combination of atomic orbitals (APW-LCAO) scheme in studies of V$_3$Si, V$_3$Ge, Nb$_3$Al, Nb$_3$Sn, and Nb$_3$Ge. The APW convergence is improved from an earlier A15 study and the LCAO

parametrization was used to obtain good k-point sampling. The approach taken by Klein et al.[8] and Arbman and Jarlborg[7] is similar in the sense that several A15's were studied by identical calculations. In the first,[8] APW, and in the second,[7] LMTO calculations carried out self-consistently, were used to search for trends among the A15 systems. The LMTO calculations used overlapping spherical potentials while the APW calculation used spherically symmetric potentials up to the interstitial region in which nonspherical corrections are made (so-called warped-tin potential approximation). The APW results of Klein et al. for the DOS used an accurate k-point integration technique and the LMTO

TABLE II. Values of λ for some transition-metal elements. Theoretical values of $\lambda_{e\text{-ph}}$ from the rigid-muffin-tin approximation (RMT) are shown and those quantities which were converted from $N(E_F)$ through Eq. (1) are listed as λ_γ. Experimental values as well as values of $\lambda_{e\text{-ph}}$ from the McMillan equation in conjunction with the empirical relation of Benneman and Garland (Ref. 43) for μ^* are also shown. The values of T_c, Θ_D, and γ which were used to calculate $\lambda_{e\text{-ph}}$ through Eq. (4) are listed in Table I.

| | Theory | | Experiment | | Empirical | |
| | RMT | Band-structure calculation | High-low temperature heat capacity | Tunneling | McMillan equation | |
Materials	$\lambda_{e\text{-ph}}$	λ_γ	λ^a	$\lambda_{e\text{-ph}}$	$\lambda_{e\text{-ph}}$	μ^*
Nb	1.22[b]	1.26[b]		1.04[c]$\pm$0.06		
	1.3[d]		0.9$\pm$0.1		0.91	0.164
	1.1[k]	1.43[d]		0.93[d]$\pm$0.1		
	0.99[o]					
La (fcc)	1.42[e]	1.42[e]			1.09	0.182
V	1.05[b]	1.07[b]				
	1.2[a]	1.09[d]	1.0$\pm$0.2	0.8[f]	0.72	0.178
				0.69[g]		
Ta	0.9[d]	1.09[d]	0.9$\pm$0.2	0.70[h]	0.74	0.154
Mo	0.34[b]	0.31[b]				
	0.4[d]	0.5[d]			0.36	0.100
	0.40[l]					
Pd	0.28[b]	0.78[b]				
	0.5[d]	0.59[d]	0.7$\pm$0.1	<0.2[n]	<0.38	
	0.41[m]	0.53[i]				
Pt	0.7[b]	0.39[d]				
		0.59[i]	0.6$\pm$0.1		<0.36	
Sc	0.64[b]	0.97[b]	0.3$\pm$0.05		<0.39	
Y	0.38[b]	1.67[b]				
		1.35[j]	0.3$\pm$0.5		<0.42	

[a]See Ref. 38.
[b]See Ref. 2.
[c]See Ref. 24.
[d]See Ref. 3.
[e]See Ref. 4.
[f]See Ref. 26.
[g]See Ref. 22.
[h]See Ref. 27.

[i]See Ref. 5.
[j]See Ref. 6.
[k]See Ref. 55.
[l]See Ref. 53.
[m]See Ref. 54.
[n]See Ref. 33.
[o]See Ref. 51.

results of Arbman and Jarlborg given here (except that of V_3Sn) were determined using a Fourier-series fitting procedure and the tetrahedron method to yield a 6-mRy energy resolution. The published LMTO DOS data[7] were determined by simple hisotogram techniques, and agree ($>90\%$) with the new Fourier-fitted tetrahedron results using an energy resolution of 10 mRy, and differ 10–20 % from the 6-mRy resolved results shown here. The

LMTO value for V_3Sn (Ref. 7) given in Table III was obtained without Fourier fitting. Both the APW (Ref. 8) and LMTO (Ref. 7) data were used for calculations of $\lambda_{e\text{-ph}}$ in the rigid-ion approximation with $\langle \omega^2 \rangle$ taken from phonon DOS of Schweiss et al.[44] data in the former[8] and from experimental Debye-temperature data in the latter[7] case. The differences between the DOS and λ values (Tables III and IV) deduced from APW and
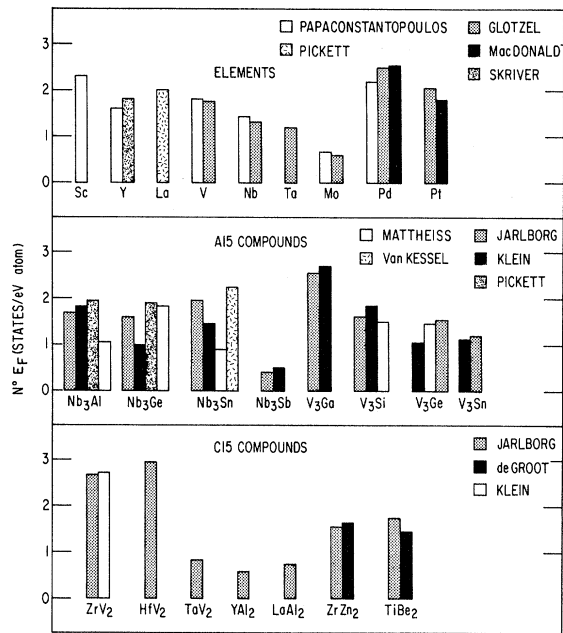
FIG. 1. Density of states $N(E_F)$ from band-structure calculations. Different calculations show good agreement with the largest discrepancies being for Nb_3Ge, Nb_3Sn, and V_3Ge.

LMTO are rather modest for some of the $A15$ compounds ($<20\%$), but can be very large ($>40\%$) for others such as Nb_3Ge and V_3Ge. The general trends, however, are quite similar with the highest DOS values found for the vanadium compounds among which V_3Ga is found by both methods to have the highest DOS among the $A15$'s considered here.

In their APW calculations on Nb_3Sn and Nb_3Sb, van Kessel et al.[11] included nonspherical contributions to the potential and used an accurate DOS determination, but did not perform the calculations self-consistently. However, dHvA data of Arko et al.[45] on Nb_3Sb showed that the Fermi-surface feature described in this calculation[11] was superior to those resulting from the "warped" APW (Ref. 8) or the LMTO (Ref. 7) results. This result can be understood to be caused by a state close to E_F which is sensitive to a nonspherical potential correction directed along the "Nb chains." The van Kessel et al.[11] DOS value comes out to be significantly larger than from the warped APW and LMTO results.

Pickett et al.[10] applied the pseudopotential method to Nb_3Ge and Nb_3Al; this calculation is both self-consistent and includes a general potential in the outer part of the atoms where nonspherical corrections are expected to be significant (however,

the pseudopotential approach is not an all-electron calculation and the effects of neglecting the core region are hard to predict). Using a rigid-band approach to determine the Fermi surface of Nb_3Sb and comparing these results[10] to the dHvA data[45] shows qualitatively again the importance of the nonspherical potential effects.

Thus, we have seen variations in the DOS results from the different calculations which are somewhat larger than for different calculations on pure metals. While the disagreement among the theoretical $N(E_F)$ for some systems have been found to be rather large, on the whole, most calculations on the $A15$'s considered here differ from the average by $\sim20\%$. Therefore, we can somewhat arbitrarily define error bars of roughly 20% for the band-calculated DOS. When comparing these theoretical results with experiment, only discrepancies which are larger than $\sim20\%$ in the values of $N(E_F)$ are considered significant.

D. $C15$ compounds

The self-consistent semirelativistic LMTO results by Jarlborg and Freeman[12] shown in Table V for the $C15$ compounds used essentially the same computation method as for the $A15$ LMTO results. The LMTO results for the $C15$'s were used to calculate $\lambda_{e\text{-ph}}$ in the rigid-ion approximation, where the values of $\langle\omega^2\rangle$ were again taken from experimental Debye-temperature data. APW results for $TiBe_2$ and $ZrZn_2$ by deGroot et al.[13] include nonspherical terms in the potential but are not self-consistent even though the potential is beyond the overlapping charge-density approximation. The DOS values for $TiBe_2$ and $ZrZn_2$ are quite similar between the two calculation methods (Fig. 1). Klein et al.[14] have performed self-consistent, semirelativistic APW calculations for ZrV_2 which agree very well with the results of Jarlborg and Freeman.[12] Results for these different calculations are shown in Fig. 1.

III. EXPERIMENTAL CONSIDERATIONS

A. Methods

The electron-phonon coupling parameter $\lambda_{e\text{-ph}}$ can be determined from a number of experiments,[46] as well as indirectly through the use of empirical methods such as that of McMillan.[41] For this study, we quote in Tables I—V values de-

TABLE III. Values of $N(E_F)$ for some $A15$ compounds. $N(E_F)$ is in units of states/cV atom both spins and γ is in units of mJ/g atom K^2. Quantities which were converted from λ values are listed as $N_\gamma(E_F)$. Values of T_c, Θ_D, and γ for these materials are also listed.

Material	T_c	γ	Θ_D	Theory Band-structure calculation $N(E_F)$	Experimental High-low temperature capacity $N(E_F)$	Tunneling $N_\gamma(E_F)$	NMR $N(E_F)$	Empirical McMillan equation $N_\gamma(E_F)$
Nb$_3$Al	18.5[a]	7.6[a]	370[a]	1.67[d] 1.83[e] 1.95[f] 1.05[g]		< 1.19[j]		1.545
Nb$_3$Ge	21.8[b]	7.58[b]	302[b]	1.60[d] 0.98[e] 1.90[f] 1.83[g]		1.22[k]		1.363
Nb$_3$Sn	17.9[a]	12.2[a]	308[a]	1.97[d] 1.45[e] 0.89[g] 2.24[h]		1.86[l]		2.274
Nb$_3$Sb	0.2[a]	1.1[a]	335[a]	0.40[d] 0.48[e]				0.369
V$_3$Si	16.5[a]	16.7[a]	498[a]	1.60[d] 1.84[e] 1.50[g]			3.86[i]	3.514
V$_3$Ga	14.3[a]	21.6[a]	399[a]	2.56[d] 2.72[e]		4.34[m]	4.28[i]	4.402
V$_3$Ge	5.8[c]	7.16[c]	470[c]	1.05[e] 1.53[d] 1.47[g]		2.03[c]		1.827
V$_3$Sn	3.8[a]	7.2[a]	364[a]	1.13[e] 1.19[d]			1.85[i]	1.864

[a]See Ref. 57.
[b]See Ref. 61.
[c]See Ref. 40.
[d]See Ref. 7; V$_3$Sn given without Fourier fitting.
[e]See Ref. 8.
[f]See Ref. 10.
[g]See Ref. 9.
[h]See Ref. 11.
[i]See Refs. 34−36.
[j]See Ref. 31; compound was off stoichiometry Nb-Al 22.8% Al ($T_c = 16.4$ K).
[k]See Ref. 32; composition was Nb$_3$Ge$_{0.81}$.
[l]See Ref. 29.
[m]See Ref. 26.

rived from comparisons of high- and low-temperature heat-capacity, tunneling, and NMR experiments. The most accurate way to obtain direct electron-phonon information is through the use of Giaever-McMillan-Rowell[47] tunneling spectroscopy techniques which allow $\alpha^2(\omega)F(\omega)$, the weighted phonon DOS, to be determined. This in turn allows $\lambda_{e\text{-ph}}$, μ^*, and other quantities of in-

TABLE IV. Values of λ for some $A15$ compounds. Theoretical values of $\lambda_{e\text{-ph}}$ from the rigid-muffin-tin approximation (RMT) are shown and those that were converted from $N(E_F)$ are listed as λ_γ. Experimental values as well as values of $\lambda_{e\text{-ph}}$ from the McMillan equation [Eq. (4)] and the empirical relation of Benneman and Garland (Ref. 43) for μ^* are shown in Table II. Values of T_c, Θ_D, and γ which were used are listed in Table III.

Material	Theory RMT $\lambda_{e\text{-ph}}$	Theory Band-structure calculation λ_γ	Experiment High-low temperature heat capacity λ	Experiment Tunneling $\lambda_{e\text{-ph}}$	Experiment NMR λ_γ	Empirical McMillan equation $\lambda_{e\text{-ph}}$	Empirical McMillan equation μ^*
Nb$_3$Al	2.14[c]	0.94[b] 0.71[c] 0.66[d] 2.08[e]		>1.7[h]±0.05		1.09	0.158
Nb$_3$Ge	1.1[b] 0.89[c]	1.02[b] 2.29[c] 0.69[d] 0.32[e]		1.64[i]±0.2		1.37	0.150
Nb$_3$Sn	1.19[c]	1.64[b] 2.58[c] 4.84[e] 1.32[f]		1.80[j]±0.15		1.30	0.181
Nb$_3$Sb	0.22[c]	0.20[b] 0.00[c]				0.28	0.070
V$_3$Si	0.9[b] 1.18[c]	3.40[b] 2.87[c] 3.74[e]			0.84[g]	1.03	0.202
V$_3$Ga	1.48[c]	2.38[b] 2.18[c]		1.12[k]	1.15[g]	1.10	0.212
V$_3$Ge	0.67[c]	1.9[c] 0.99[b] 1.07[e]	0.5[a]			0.67	0.168
V$_3$Sn	0.52[c] 0.6[b]	1.72[c] 1.60[b]			0.66[g]	0.65	0.169

[a]See Ref. 40.
[b]See Ref. 7; V$_3$Sn given without Fourier fitting.
[c]See Ref. 8.
[d]See Ref. 10.
[e]See Ref. 9.
[f]See Ref. 11.
[g]See Refs. 34−36.
[h]See Ref. 31; compound was off-stoichiometry Nb-Al 22.8% Al ($T_c = 16.4$ K).
[i]See Ref. 32; composition was Nb$_3$Ge$_{0.81}$.
[j]See Ref. 29.
[k]See Ref. 26.

terest to be determined. Much of the tunneling data quoted below has only recently become available. Advances, due to Arnold,[48] which take into account proximity layers, both intentionally and unintentionally introduced, have greatly increased the availability of information concerning the electron-phonon interaction for the transition-metal elements and the $A15$ compounds. For transition-

TABLE V. Values of λ and $N(E_F)$ for some $C15$ compounds. $N(E_F)$ is in units of states/eV atom both spins and γ is in units of mJ/g atom K^2. Theoretical values of $\lambda_{e\text{-ph}}$ from the rigid-muffin-tin (RMT) approximation are shown and values of λ converted from $N(E_F)$ are listed as λ_γ. Values from the McMillan equation [Eq. (4)] and the empirical relation of Benneman and Garland (Ref. 43) for μ^* are shown along with T_c, Θ_D, and γ values that were used.

Material	T_c	γ	Θ_D	RMT $\lambda_{e\text{-ph}}$	Theory Band-structure calculation		μ^*	Empirical McMillan equation $N_\gamma(E_F)$	$\lambda_{e\text{-ph}}$
					λ_γ	$N(E_F)$			
HfV$_2$	8.85[a]	17.9[a]	255[a]	3.03[b]	1.74[b]	2.95[b]	0.206	3.71	1.055
ZrV$_2$	8.80[c]	16.5[b]	290[b]	2.40[b]	1.62[b]	2.68[b]	0.203	3.53	0.99
					1.57[e]	2.73[e]			
TaV$_2$	3.58[a]	9.6[a]	350[a]	0.66[b]	3.76[b]	0.86[b]	0.189	2.43	0.69
LaAl$_2$	3.29[h]	3.65[h]	352[h]	0.40[b]	1.10[b]	0.74[b]	0.133	1.02	0.55
YAl$_2$	<0.05[h]	1.81[h]	473[h]	0.15[b]	0.30[b]	0.59[b]		>0.264	<0.264
ZrZn$_2$		12.9[f]	370[b]		2.54[b]	1.55[b]			
					2.39[d]	1.62[d]			
TiBe$_2$		13.7[g]	650[g]	0.54[b]	2.39[b]	1.72[b]			
					3.02[d]	1.45[d]			

[a]See Ref. 56.　　　　　　　　　　　　[e]See Ref. 14.
[b]See Ref. 12.　　　　　　　　　　　　[f]See Ref. 63.
[c]See Ref. 62.　　　　　　　　　　　　[g]See Ref. 64.
[d]See Ref. 13.　　　　　　　　　　　　[h]See Ref. 65.

metal elements, recent tunneling data due to Wolf et al. are available for Nb,[23,25] V,[26] and Ta,[27] and Dunoulin et al.[33] have reported a new measurement on Pd. Knapp and co-workers[37–39] have determined λ for V, Nb, Ta, Pt, Pd, Sc, and Y metals from the comparison of heat-capacity data at high and low temperatures. The accuracy of these determinations is $\sim \pm 20\%$. The tunneling results on Nb, V, and Ta agree (within error limits) with the heat-capacity determinations, while the $\lambda_{e\text{-ph}}$ value derived for Pd from tunneling is much lower. This difference is understood since spin fluctuations are known to be very important in Pd. Recall that the tunneling data measures $\lambda_{e\text{-ph}}$ while the high- and low-temperature heat capacity measures the total mass enhancement $\lambda = \lambda_{e\text{-ph}} + \lambda_{\text{spin}}$. Comparing the two values gives $\lambda_{\text{spin}} \gtrsim 0.5 \pm 0.1$. In the case of Pd it is clear that λ_γ derived from the band-structure results should be compared only to the high- and low-temperature heat-capacity result.

For the $A15$ compounds,[49] NMR results of Fradin et al.[34–36] give the bare DOS at the Fermi level, $N(E_F)$, to an accuracy of $\sim 30\%$. For the vanadium-base $A15$'s values are reported for V$_3$Si,[35] V$_3$Ga,[35] and V$_3$Sn.[34] Tunneling data is available for V$_3$Ga,[26] Nb$_3$Al,[31] Nb$_3$Sn,[29] and Nb$_3$Ge.[32] For V$_3$Ge, Panova et al.[40] report a λ value based on the

method of comparison of high- and low-temperature specific heat. Note that for V$_3$Ga, the two results of the independent measurements given in Table IV agree within the experimental error. For the $C15$ compounds, there are as yet no direct experimental determinations of λ.

B. McMillan equation

The McMillan equation, which relates T_c to a phonon energy Θ_D, an electron-electron interaction energy μ^*, and $\lambda_{e\text{-ph}}$, is given in Eq. (4). Allen and Dynes[42] have shown that for materials with $\lambda_{e\text{-ph}} < 1.5$, the McMillan equation is accurate if $\Theta_D/1.45$ is replaced by $\langle \omega \rangle / 1.20$, where

$$\langle \omega \rangle = \frac{2}{\lambda} \int_{e\text{-ph}}^{\infty} d\omega \, \alpha^2(\omega) F(\omega) \tag{6}$$

and

$$\lambda_{e\text{-ph}} = 2 \int_0^\infty \frac{d\omega \, \alpha^2(\omega) F(\omega)}{\omega} . \tag{7}$$

The McMillan equation values of $\lambda_{e\text{-ph}}$ shown in Fig. 2 and Tables II, IV, and V have been computed using $\Theta_D/1.45$, which allows us to compare in a consistent manner the $\lambda_{e\text{-ph}}$ values derived for the $C15$ and some $A15$ materials where detailed tunnel-

ing data and therefore $\langle \omega \rangle$ is not yet available. For μ^*, we use the formula of Benneman and Garland,[43] Eq. (5), where $N(E_F)$ is made consistent with the McMillan equation in an iterative procedure. A measure of the error introduced by using Θ_D instead of a more appropriate average over the phonon DOS can be seen from the values quoted by Allen and Dynes[42] for both methods; approximately a $10-15\%$ variation is noted. Since the errors which are involved in the calculations of λ from $N(E_F)$ and γ through Eq. (1) are at least of this order of magnitude, the use of the less accurate form of the McMillan equation does not pose a serious problem for this application. The difference in λ values between theory and experiment, which will be discussed in Sec. IV, far exceed the reasonable limits which can be placed on the McMillan equation values for most of these materials.

A comparison between the values of $\lambda_{e\text{-ph}}$ derived through the McMillan equation, and from experimental determinations is shown in Fig. 2. For the metals the agreement is very good, with the McMillan equation giving values closest to those from tunneling measurements. For the vanadium $A15$'s the agreement is also good. The Nb_3X compounds, however, show a marked disagreement between the values from tunneling and those from the McMillan equation. This disagreement arises from the need to use a more accurate form of the McMillan equation[42] for materials having values of $\lambda_{e\text{-ph}} > \sim 1.5$. For the $C15$'s where no independent experimental values exist, the McMillan equation yields $\lambda_{e\text{-ph}}$ values less than or equal to 1, and so is expected to be accurate to approximately the same
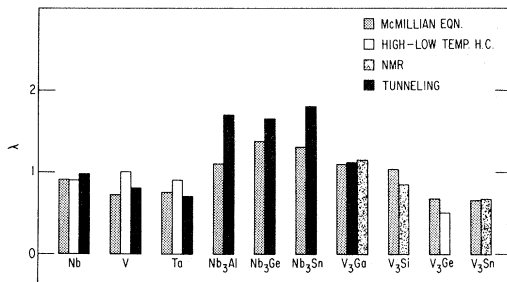

FIG. 2. Comparison of the McMillan equation [Eq. (4)] to all available experimental values. McMillan values were derived using $\mu^*=0.26N(E_F)/1+N(E_F)$ and the values of T_c, Θ_D, and γ listed in Tables I–III. Good agreement is seen with the exception of Nb$_3$Al, Nb$_3$Ge, and Nb$_3$Sn, where the McMillan values differ significantly from the tunneling data.

level as the V $A15$'s which have λ values of the same order of magnitude.

IV. COMPARISON OF BAND-STRUCTURE PREDICTIONS AND EXPERIMENT

In order to compare results from different band-structure results, all values of $N(E_F)$ from different workers have been converted to states/eV atom both spins.

Tables I–V contain values of both $N(E_F)$ and λ for the band-structure, experimental, and McMillan results. Values of $N(E_F)$ have been converted through Eq. (1) to λ values [and λ values to $N(E_F)$] for comparison purposes. Values of $\lambda_{e\text{-ph}}$ derived from the RMT approximation have not been converted to a DOS value. Note that the relative errors resulting from comparing λ values is approximately twice the errors resulting from comparing the values of $N(E_F)$, which compares $1+\lambda$ rather than λ itself. The percent difference, Δ defined as $100(\lambda_{\text{theor}}-\lambda_{\text{expt}})/\lambda_{\text{expt}}$ is shown for the λ values in Table VI.

A. Transition-metal elements

In Table I five superconducting elements, Nb, V, Ta, Mo, and fcc La, as well as Pd, Pt, Sc, and Y, which are not superconducting at normal pressures, have been included. The band-structure results are shown for all the materials in Fig. 1. The different band-structure results for the transition-metal elements are fairly consistent for different workers and approximations. The different experimental results also agree very closely as discussed in Sec. III. Among the superconducting elements considered, differences between theory and experiment ranged from $\sim 5\%$ for Mo to $\sim 20\%$ for Nb and V (see Fig. 3). These types of differences are within the error bars discussed in Secs. II and III. For the nonsuperconducting elements, the results for Pt and Pd agree within the error limits, while those for Sc and Y differ markedly.

The discrepancies found for Sc and Y are possibly connected with spin fluctuations in these elements. Spin fluctuations or "paramagnons" involve the alignment of electron spins, and so act to lower T_c through a pair-breaking effect.[1] Paramagnons have been shown to totally suppress T_c in Pd,[50] and could be important in other transition metals as well.[1] For example, both Pd and Pt are found to have mass enhancement values[38]

TABLE VI. Percent difference Δ between theory and experiment for λ.
$\Delta = 100(\lambda_{\text{theor}} - \lambda_{\text{expt}})/\lambda_{\text{expt}}$, where experimental values have been averaged if more than one exists. Where no experiments were available, values from the McMillan equation [Eq. (4)] were used. Note that when there are large differences, the theory is usually below the experimental values.

Elements		$A15$		$C15$	
Sc	$+223\%^{a}$	Nb$_3$Al	$-44\%^{f}$	ZrV$_2$	$+64\%^{k}$
			$-58\%^{g}$		$+59\%^{l}$
Y	$+450\%^{a}$		$-61\%^{h}$		
	$+350\%^{e}$		$+23\%^{i}$	HfV$_2$	$+65\%^{k}$
		Nb$_3$Ge	$-38\%^{f}$		
La	$+30\%^{c}$		$+40\%^{g}$	TaV$_2$	$+445\%^{k}$
			$-58\%^{h}$		
V	$+21\%^{b}$		$-53\%^{i}$	LaAl	$+110\%^{k}$
	$+19\%^{a}$				
		Nb$_3$Sn	$-9\%^{f}$		
Nb	$+49\%^{b}$		$+43\%^{g}$		
	$+34\%^{a}$		$+169\%^{i}$		
			$-27\%^{j}$		
Ta	$+42\%^{b}$				
		Nb$_3$Sb	$-29\%^{f}$		
Mo	$+39\%^{b}$		$-100\%^{g}$		
	$-13\%^{a}$				
		V$_3$Ga	$+110\%^{f}$		
Pd	$+11\%^{a}$		$+92\%^{g}$		
	$-16\%^{b}$				
	$-24\%^{d}$	V$_3$Si	$+305\%^{f}$		
			$+242\%^{g}$		
Pt	$-35\%^{b}$		$+205\%^{i}$		
	$-29\%^{d}$				
		V$_3$Ge	$+280\%^{g}$		
		V$_3$Ge	$-98\%^{i}$		
			$-114\%^{f}$		
		V$_3$Sn	$+163\%^{g}$		
			$+144\%^{f}$		

[a]See Ref. 2.　　　　　　　　　　[g]See Ref. 8.
[b]See Ref. 3.　　　　　　　　　　[h]See Ref. 10.
[c]See Ref. 4.　　　　　　　　　　[i]See Ref. 9.
[d]See Ref. 5.　　　　　　　　　　[j]See Ref. 11.
[e]See Ref. 6.　　　　　　　　　　[k]See Ref. 12.
[f]See Ref. 7.　　　　　　　　　　[l]See Ref. 14.

which would give superconductivity in the McMillan theory. These large λ's (0.7 for Pd and 0.6 for Pt) can be reconciled with the experimental absence of superconductivity if spin fluctuations are included. Recent proximity tunneling measurements of Dumoulin et al.[33] on Pd give $\lambda_{e\text{-ph}} < 0.2$, which would explain the absence of superconductivity. The additional contribution to λ is caused by spin-fluctuation effects. Recent calculations of λ_{spin} by MacDonald give values for Sc and Y of 0.71 and 0.45, respectively. The question of spin fluctua-

tions has also arisen recently[19] for Nb and V. The values of λ_{spin} were determined by Rietschel and Winter by considering the differences between their calculated values of $\lambda_{e\text{-ph}}$, and the λ values derived from theoretical DOS and heat-capacity results. These differences, and therefore λ_{spin}, are not, however, outside the error bars discussed in Sec. II B for the band-structure calculations on these materials.

The discussion above did not include the $\lambda_{e\text{-ph}}$ values calculated from the RMT approximation.

For the transition-metal elements, these calculations[2,3,51−55] are shown in Table II. The RMT approximation appears accurate to about the same level as do the results obtained from band-structure DOS and specific-heat data. The RMT calculations do somewhat better for Pd and Y, while doing worse for Pt and Sc.

B. $A15$ and $C15$ compounds

The relevant $N(E_F)$ values for the $A15$ compounds are shown in Table III and Fig. 1. The values obtained from different calculations are again fairly consistent, though much less so than in the elements, and a wide variation is seen in the values V_3Ge and Nb_3Sn and Nb_3Ge. The McMillan equation appears to agree with experiment for V_3X compounds, while the large disagreements seen for Nb_3Al, Nb_3Sn, and Nb_3Ge are discussed in Sec. V. In general, the disagreements between theory and experiment are worse for the $A15$ materials than for the transition-metal elements (see Fig. 3). The discrepancies in the values of λ are 100% or worse for some $A15$ materials such as V_3Si and V_3Sn. The results for the Nb-based $A15$'s are much better than the V based, though some variation is seen. The V_3X compounds show disagreements that are far outside reasonable errors for either the experimental or theoretical determinations of λ.

Recent work by Orlando and Beasley[20] have shown that spin fluctuations are more important in $A15$ compounds than previously thought. By considering the range of experimental parameters, they arrive at a range of values for λ_{spin}. For V_3Ga and V_3Si, their maximum estimate of $\lambda_{spin}=0.30$ helps to bring the theory and experiment together, but still leaves a significant part of the discrepancy unaccounted for.

The $C15$ materials have been much less studied than the $A15$ compounds, and as yet no direct experimental determinations of λ or $\lambda_{e\text{-ph}}$ have been performed. Keeping in mind the level of agreement found between the McMillan equation and experiment for the $A15$'s, we can still get a feeling for how well theory is doing in calculating λ for these materials. The data for the $C15$'s is presented in Table V. The differences in λ values calculated from theoretical DOS for HfV_2, ZrV_2, and those from the McMillan equation range from 60−70%. Since the McMillan-equation values of $\lambda_{e\text{-ph}}$ are of an order of 1 or less, we expect that their accuracy should be similar to that found for the V_3X compounds. HfV_2 and ZrV_2, however, are not cubic at low temperatures, which was not included in the calculation. Both materials undergo a phase transition from cubic to lower symmetry at temperatures above 100 K. Susceptibility results[56] indicate that "cubic" HfV_2 and ZrV_2 would have much higher γ values if they stayed cubic, a fact which would decrease the discrepancy. TaV_2 and $LaAl_2$, however, which do not transform, show differences in λ between the McMillan equation and calculations of 300−400%, respectively. These discrepancies are outside of the estimated error limits, considering the level of accuracy assigned to the McMillan equation determination of $\lambda_{e\text{-ph}}$. The results for $YA1_2$, $ZrZn_2$, and $TiBe_2$ have been included for completeness, though no comparisons with experiment are possible.

The RMT values (shown in Table IV) agree closely with experiment or McMillan equation values for the low-T_c $A15$ compounds, but differ markedly for the high-T_c $A15$'s. In the $C15$ materials, the RMT does well for $LaAl_2$ and TaV_2, while for HfV_2 and ZrV_2, large discrepancies are found from the RMT $\lambda_{e\text{-ph}}$'s and those from the McMillan equation. The large discrepancies are at least primarily caused by the fact that RMT $\lambda_{e\text{-ph}}$ values were calculated for the cubic phase whereas at low temperatures HfV_2 and ZrV_2 have lower symmetry. Heat-capacity results[56] show that the lattice hardens markedly below T_c for both materials.

V. DISCUSSION

From the discussion in the last section it is clear that large disagreements between the determinations of λ from theoretical DOS and γ values and those from experiment or the McMillan equation exist for some of the materials we are considering. This is particularly evident for the vanadium-based $A15$'s, TaV_2, $LaAl_2$, Sc, and Y. There are also problems in the niobium-based $A15$'s, but the situation here is less clear with these compounds seeming to fit in a somewhat different category from the vanadium-based $A15$'s. The band-structure results are less consistent, and the discrepancies, as shown in Table VI, are less severe than for the V $A15$'s. Some of the band-structure calculation determinations of λ are in fairly good agreement with those from experiment or using the McMillan equation.

Recent tunneling measurements of Nb_3Sn, Nb_3Al, and Nb_3Ge found very high values of $\lambda_{e\text{-ph}}$ (>1.6), which are much higher than expected from
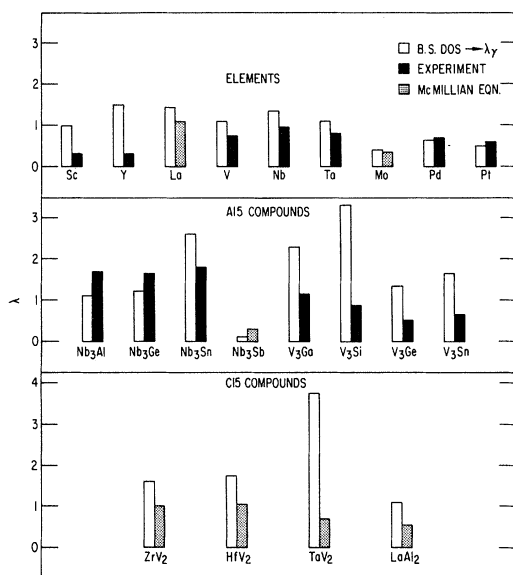
FIG. 3. Comparison of experimental and theoretical values of λ. Where more than one value exists, the average is shown in the graph. For many of the materials shown, serious discrepancies can be seen and are discussed in the text. RMT values are not included.

the McMillan equation. This is in contrast to the vanadium-based A15's ($\lambda_{e\text{-ph}} \leq 1$) where, for example, in V_3Ga, $\lambda_{e\text{-ph}}$ values from tunneling, NMR, and the McMillan equation all agree within 10% or better. Also, in contrast to the general trend, most of the band-structure DOS results are too high with respect to the experimental values for the Nb_3X compounds and the new tunneling results only increase this discrepancy (see Fig. 3). For all the other materials where the discrepancies are significant, the band structure DOS is too *low*, giving a λ value which is too high with respect to experimental or the McMillan-equation values. One final difference to mention is the correlation between DOS and λ, which is evident for the vanadium A15's and does not exist for the niobium-based A15 compounds.[58,59]

For the vanadium-based A15's, C15's, Sc, and Y, we are left with serious disagreements become theory and experiment of 60–450%. In these materials, the band-structure results are consistent for different approximations. Experimentally for the C15's, we have only the McMillan equation while for the A15's, we have some independent results from tunneling, NMR, and high-low temperature comparisons of specific heat. In most cases where we have more than one independent experimental result for λ, they agree both with each oth-

er and the McMillan equation. Thus, both the experimental and theoretical values are fairly consistent within themselves, and the disagreements we are discussing are outside the reasonable error bars of both. In all these cases, the theoretically determined values of $N(E_F)$ are too low, compared with experiment. As was mentioned in Sec. III, the calculations reviewed here are for perfect crystals, and do not take into account lattice imperfections, nonstoichiometry, or subtle lattice transformations. These effects, however, would usually only serve to decrease the discrepancies between theory and experiment. For the high-DOS materials, removing the imperfections or transformations generally raises the λ values. It is especially important to consider this point for the A15 and C15 compounds since ZrV_2, HfV_2, V_3Si, and Nb_3Sn do undergo phase transitions from cubic to lower symmetry which may lead to a decrease of $N(E_F)$. Further, a high DOS also leads to increased Stoner factors, which determines, if not the onset of a magnetic state, a state where spin fluctuations become important. This effect is more pronounced when the local DOS is considered rather than the total DOS per unit cell divided by the number of atoms as a measure of the DOS. In particular since the A15 compounds have a larger local DOS on the transition-metal sites (V or Nb), some of the quantities discussed would be modified and also be of increased importance for estimates of Stoner factors in the "nearly magnetic" materials. However, Stoner factors (and thus probably also spin fluctuations) are comparatively less important in Nb-based or other $4d$ superconductors, because apart from the contribution from the local DOS, the localized $4d$ wave functions give smaller exchange-correlation contributions to the Stoner factor than do the $3d$ electrons.

One can view these discrepancies as arising from any or all of the following possibilities:

First, that the theoretical $N(E_F)$ values are too low for some unknown reason such as the use of incorrect local density potentials, or numerical inaccuracies in the calculations. This would imply something general about the band calculations, since for these materials the different calculations are all consistent.

Second, one could question the experimental or empirical evidence. Certainly in the cases where the McMillan equation is not supported by independent values, one could question its applicability to these systems. A particular example of this is the C15's. For the Nb-based A15's there are serious discrepancies between the McMillan equa-

tion and the tunneling results due to the fact that Eq. (4) becomes increasingly less accurate for λ values ≥ 1.5. For the vanadium-based $A15$'s, the McMillan values agree fairly well with the available experimental evidence and are expected to be of similar accuracy for the $C15$'s, which also have λ values $\lesssim 1$.

Third, one can assume that in these systems spin fluctuations are important. They are known to be important in Pt and Pd where they are effective in suppressing superconductivity. There is a possibility that strong spin fluctuations exist in Sc and Y as well. Spin fluctuations have been shown to be non-negligible in some $A15$ compounds,[20] however, even assuming the maximum estimate for λ_{spin}, the large differences are not completely diminished. Whatever mechanisms are actually involved, these

discrepancies indicate that some important problems remain to be solved in these materials.

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