ELECTRONIC STRUCTURE, ELECTRON-PHONON INTERACTION AND HIGH-TEMPERATURE SUPERCONDUCTIVITY IN V₃Si

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Using the results of our self-consistent APW band structure calculations, we have calculated the electron-phonon interaction, n(Γ₂), the electron mass enhancement factor λ, and the superconducting transition temperature Tc for V₃Si. Our results are in good agreement with the experimental values. In addition we find that the band structure results are a) in good qualitative agreement with the non-self-consistent results of Mattheiss, and b) show no detailed verification for any of the one-dimensional models of the electronic properties of the A15 materials.

1 INTRODUCTION

There has been great experimental and theoretical interest in the A15 materials (A₃B) in recent years. Several of these compounds have the highest superconducting transition temperatures (Tc) known, and in addition these materials are noted for their anomalous low-temperature electrical, magnetic and elastic properties. Furthermore, V₃Si and Nb₃Sn undergo structural phase transitions at temperatures somewhat above Tc. Details of the work done on the A15 materials have been discussed in three recent review articles.¹⁻³

Theoretical work on these materials has focused on a proposed unusually sharp peak in the density of states (DOS) at the Fermi energy, E_F. These include the models of Clogston and Jaccarino,⁴ Labbé and Friedel,⁵ Cohen, et al.,⁶ and Gor'kov.⁷ Weger and co-workers (see Ref. 1) have attempted to give a detailed justification of the Labbé-Friedel model, which exploits the linear-like packing of the A-atoms in the A15 structure. Mattheiss has performed non-self-consistent APW calculations for several A15 materials⁸,⁹ and finds a large DOS at E_F, but no detailed justification for any of these one-dimensional models.

In this work we use the results of our self-consistent (SC) APW band structure calculations,¹⁰ to compute the electron-phonon interaction, mass enhancement factor λ, and Tc of V₃Si. The plan of the paperting paper is as follows: in Section II we discuss the SC band structure calculation and results; in Section III we formulate and present results for the electron-phonon and Tc calculations; and in Section IV we present our conclusions.

2 BAND STRUCTURE RESULTS

The band structure energies and wave functions—of V₃Si have been computed¹⁰,¹¹ using the self-consistent APW method¹² with the xα local exchange approximation.¹³ The vanadium (3s 3p 3d 4s) and the silicon (3s 3p) states were treated as bands, while the inner “core” states were recomputed “atomic-like” in each cycle. The self-consistency procedure consisted of the following steps: 1) atomic charge densities were used to construct initial starting muffin-tin potentials for the V and Si sites; 2) energies and wave functions were computed on a uniform mesh in k-space in the 1/48 irreducible cubic Brillouin zone, equivalent to 64 k-points in the full zone; 3) states were filled with the V and Si electrons, and muffin-tin charge densities and potentials were constructed from the occupied Bloch states; 4) steps 2 and 3) were repeated until there was convergence between two successive cycles. For V₃Si four cycles were performed, with a measure of the excellent convergence achieved being the fact that the maximum difference in energy of a given state between cycles three and four was ~1 mRy (10⁻⁴ eV). In essence, the V₃Si band structure was done in the standard APW manner—but on a “massive” scale due to the 38 valence electrons in the unit cell, and the complexities of the non-symmetric A15 space group (O₃h). Full details of the band structure calculation will be given elsewhere,¹¹ but here we will comment on some of the more important results.

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ELECTRONIC STRUCTURE, ELECTRON-ION INTERACTION AND
HIGH-TEMPERATURE SUPERCONDUCTIVITY IN YBa$_2$Cu$_3$O$_x$

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1. INTRODUCTION

The recent discovery of the superconducting state in yttrium-barium-copper-oxide (YBCO) systems has rekindled interest in the physics of these materials. The high transition temperatures ($T_c$) observed in YBCO compared to traditional superconductors has led to significant theoretical and experimental efforts to understand the nature of the superconducting state in these materials.

2. BACKGROUND

Historically, superconductivity was first observed in the 1930s in mercury, lead, and tin. Since then, superconductivity has been observed in a wide range of materials, each with its own unique properties. The physics of superconductivity is still an active area of research, with new materials being discovered and existing materials being re-examined.

3. EXPERIMENTAL RESULTS

Recent experiments have shown that the superconducting state in YBCO can be achieved at temperatures above 90 K, which is significantly higher than the 30 K transition temperature of the previous record holder, lead. These higher transition temperatures have led to a surge of interest in the potential applications of these materials, including in the development of new electrical devices.

4. THEORETICAL MODELS

The theoretical models used to describe the superconducting state in YBCO are based on the BCS theory, which was developed to explain superconductivity in traditional metals. However, the high transition temperatures observed in YBCO suggest that additional factors may be at play, such as the presence of magnetic interactions or the role of charge carriers.

5. CONCLUSIONS

The recent discovery of superconductivity in YBCO has opened up new avenues of research in the field of condensed matter physics. The high transition temperatures observed in these materials have the potential to revolutionize the field of superconductivity, and continued research in this area is expected to lead to new discoveries and applications.
induce shifts in an energy state of up to ~10 mRy. These corrections cannot significantly alter our SC results.

It was felt by some that self-consistency might have a serious qualitative effect on the states near $E_F$ (see for instance Ref. 1). Weger and Goldberg considered that SC corrections might move the bands so that $E_F$ would fall near the lower $\Gamma_{25}$ state in Figure 1, and add quantitative validity to the Labbé-Friedel type of one-dimensional band structure. However, we find that $\Gamma_{25}$ falls 60 mRy (0.84 eV) below $E_F$.

The Gorkov model for the A15 structure depends on a state at the X-point being very close to $E_F$. We find that the nearest X-point state falls 27 mRy (0.37 eV) below $E_F$. In both cases, especially with regard to the $\Gamma_{25}$ state, we don't feel that any of the remaining corrections to the SC calculations (for instance correlation effects or non-muffin-tin corrections) will bring the SC band structure calculations into quantitative agreement with these models.

Therefore, with the ~10 mRy accuracy of the SC band structure calculations, there is not any justification for treating the electronic structure of $V_3$Si as one-dimensional.

3 ELECTRON-PHONON INTERACTION

Gaspardi and Gyorffy have derived an expression for the average electron-phonon ($e-p$) interaction which is given by

$$n \langle I^2 \rangle = \frac{E_F}{\pi^2 n} \sum_{l=0}^{\infty} 2(l+1) \sin^2(\delta_{l+1}^\kappa - \delta_l^\kappa) \frac{n_{l+1}^\kappa n_l^\kappa}{N_{l+1} N_l}$$

(1)

Here $k$ labels an atom in the unit cell, V or Si in our case; $n$ is the total DOS, and $n_{l}^\kappa$ is the DOS decomposed by site and angular momentum $l$, both evaluated at $E_F$; $\delta_l^\kappa$ are scattering phase shifts; and $N_{l}^\kappa$ are “free-scatter” DOS defined in Ref. 16. It was shown by John that Eq. (1) is exact for cubic crystals within the muffin-tine approximation; while Boyer, Klein and Papaconstantopoulos have shown that certain non-muffin-tin approximations are included in calculations for transition metals based on Eq. (1).

In Table 1 we give the values of the DOS and $\langle I^2 \rangle$ which follow from our SC calculations and Eq. (1). It is quite striking that $\langle I^2 \rangle_V$ is some two-hundred times greater than $\langle I^2 \rangle_{Si}$. This is primarily due to the much larger DOS for the V sites compared
ELF-TECHNIQUES FOR PLOWCOMING

2 ELECTRON-MOLECULE INTERACTIONS

Consider the following equation for electron-molecule interactions:

\[ (\alpha + \beta)^2 = \gamma \]

where \( \alpha, \beta, \) and \( \gamma \) are parameters relevant to the interaction.

This equation is used to model the behavior of electrons interacting with molecules in various environments.

Typically, parameters \( \alpha, \beta, \) and \( \gamma \) are determined through experimental data and theoretical calculations, providing insights into the electronic structure and dynamics of the system.
Table 1

Table I: Total and angular momentum and site decomposed densities of states for V$_2$Si, and average electron-phonon interaction $n(I^2)$ for V$_2$Si

<table>
<thead>
<tr>
<th>Energy (Ry)</th>
<th>$n_s$</th>
<th>$n_p$</th>
<th>$n_d$</th>
<th>$n_f$</th>
<th>$n(I^2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>States/Ry/unit cell/spin</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>0.636</td>
<td>4.690</td>
<td>83.950</td>
<td>0.492</td>
<td>9.5</td>
</tr>
<tr>
<td>Si</td>
<td>0.149</td>
<td>1.593</td>
<td>1.890</td>
<td>0.142</td>
<td>0.40</td>
</tr>
</tbody>
</table>

For a monatomic material, it is straightforward to evaluate the mass-enhancement factor $\lambda$ from the calculated $n(I^2)$ and the measured phonon spectrum. McMillan$^{19}$ showed that in the "constant $\alpha^2$" approximation,

$$\lambda = \frac{n(I^2)}{M(\omega^2)}$$

with $M$ the atomic mass and $\langle \omega^2 \rangle$ a moment of the phonon DOS. Klein and Papaconstantopoulos$^{20}$ have formulated an extension of Eq. (2) for diatomic materials where one constituent is much heavier than the other. Since vanadium is almost a factor of two heavier than silicon, and in addition there are three times as many vanadium as there are silicon atoms in the unit cell of V$_2$Si, we follow Ref. 20 and write,

$$\lambda_{V, Si} = \frac{n(I^2)_{V, cell}}{M_\text{V} \langle \omega^2 \rangle \text{acoustic}}$$

Figure 2: Total and two decomposed densities of states for V$_2$Si based on the self-consistent APW results obtained using the "QUAD" method, Ref. 14. The scale for the integrated total density of states is shown on the right in the upper part of the figure.
TABLE II

<table>
<thead>
<tr>
<th></th>
<th>(\lambda) (calc.)</th>
<th>(\lambda) (expt.)</th>
<th>(T_c) (calc.)</th>
<th>(T_c) (expt.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V_3)Si</td>
<td>1.28</td>
<td>1.14</td>
<td>20.4 K</td>
<td>17.1 K</td>
</tr>
</tbody>
</table>

where \(n(I^2)_\text{cell}\) is for the six V atoms in the unit cell (as in Table I), and we have dropped the term for Si, as we see from Table I that \(n(I^2)_\text{Si}\) is negligible, while the denominator would be about the same as the V term in Eq. (3). Fortunately this should be a good approximation for \(V_3\)Si, as only the acoustic mode part of the phonon DOS has been measured! Finally, we calculate \(T_c\) using the Allen and Dynes\textsuperscript{21} modification to McMillan’s\textsuperscript{19} equation,

\[
T_c = \frac{f_1 f_2 \omega^2_{\text{log}}}{1.2} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.02\lambda)}\right)
\]

(4)

where \(f_1, f_2\) and \(\omega^2_{\text{log}}\) are defined in Ref. 21. We alert the reader that in the notation of Ref. 21, \((\omega^2)^{1/2} = \omega_2\).

The phonon moments have been obtained from the neutron measurements of Schweiss\textsuperscript{22} and are given by:

\[
(\omega^2)^{1/2} = 293.6 \text{ K}
\]

(5)

\[
\omega^2_{\text{log}} = 215.9 \text{ K}
\]

In addition, we have used the value \(\mu^* = 0.13\) in our calculation.\textsuperscript{19} The results are shown in Table II, where we see that the calculated values of \(\lambda\) and \(T_c\) are in good agreement with the experimentally determined values.\textsuperscript{23}

We have not attempted to institute any of the corrections to the muffin-tin approximation discussed in Ref. 18 for two reasons: 1) the lack of great accuracy in our DOS values precludes making such subtle corrections for \(V_3\)Si; and 2) in any case, we know of no rigorous way, at present, of applying these corrections to compounds. Our best estimate is that our calculated \(\lambda = 1.28\) is a reliable upper bound. A more accurate DOS calculation, and non-muffin-tin corrections, may lower \(\lambda\) by 25%.

IV CONCLUSIONS

We conclude that the standard SC APW method, and the Gaspary-Gyorgy electron-phonon theory,\textsuperscript{16-17} gives a very adequate representation of the electron-phonon interaction and mass enhancement factor \(\lambda\) for \(V_3\)Si, and most likely the other Al5 materials as well. In essence, \(V_3\)Si behaves like a “super vanadium”, with the DOS at \(E_F\) for the V atom being about twice the value of vanadium metal.\textsuperscript{18} The SC band structure results indicate that the various one-dimensional models are merely a parameterization of this fact, and should not be taken literally.

ACKNOWLEDGMENTS

We gratefully acknowledge a collaboration with L. F. Mattheiss on the band structure calculation. The phonon moments of \(V_3\)Si were calculated from Schweiss’ data by J. Hui, and were kindly communicated to us by P. B. Allen. We acknowledge computer support from Argonne National Laboratory, and helpful conversations with F. M. Mueller.

REFERENCES

18. L. I. Boyer, B. M. Klein and D. A. Papacostantinopoulos (to be published).
20. B. M. Klein and D. A. Papacostantinopoulos (to be published).
23. \(\lambda\) (expt.) was evaluated using Eqs. 4 and 5 and the value of \(T_c\) (expt.).