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First-principles determination of superconducting properties of metals

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Abstract

Ab initio and many-body-theory methods are combined to determine the coupling of electrons to phonons in real materials. The electron-phonon spectral function is determined using a linear-response technique within density functional theory, and superconducting properties are then extracted with Migdal–Eliashberg theory. We examine the puzzle of a low T_c in Li and determine theoretical estimates for T_c in high-pressure phases of sulphur, which is the highest transition temperature elemental superconductor. These examples show that theoretical calculations are reaching a stage where their accuracy is now competitive with that of experiments. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: High-pressure sulphur

1. Introduction

First-principle density-functional theories [1,2] can now be employed to calculate band-structures, phonon dispersions, and the electron–phonon spectral function $\alpha^2F(\Omega)$ which measures how efficient phonons of energy Ω scatter electrons within the Fermi surface. Accurately determined α^2Fs can then be employed to estimate superconducting properties of many real materials. We report on the progress made in the theoretical examination of two materials, Li and S, which are difficult systems to measure experimentally, and which exhibit puzzling behaviour.

2. Lithium

Lithium crystallizes in a body-centred-cubic (BCC) structure at room temperature, but has a phase transition to a 9R close-packed structure at a temperature of about 80 K. Earlier theoretical calculations have estimated the coupling of electrons to phonons in BCC Li to be similar to that seen in Al, but while Al superconducts at 1.1 K, no superconductivity has been observed [3,4] in Li down to 6 mK.

Our results [5] for α^2F in both the 9R and BCC phases are shown in Fig. 1 along with a plot of T_c versus the Coulomb pseudopotential evaluated at the maximal phonon frequency $\mu^*(\Omega_{max})$. The electron–phonon coupling is weaker in the 9R phase ($\lambda = 0.34$) than in the BCC phase ($\lambda = 0.45$). The maximum value of μ^* for Li can be estimated from the Anderson–Morel formula and the Fermi energy and Debye temperature as $\mu^*_{max} = 1/\ln(E_f/\Theta_D)$ which is 0.23 for Li. The inset to Fig. 1 shows our theoretical prediction for 9R Li which should have a superconducting T_c larger than 1 mK and a Coulomb pseudopotential that satisfies $\mu^* \approx 0.2$.

3. Sulphur

Sulphur is a good insulator at ambient pressure, but under compression it undergoes a series of structural phase transitions, and metallizes. Measurements [6] have shown it to be the highest T_c elemental superconductor with $T_c \approx 17$ K when it transforms to the β-Po phase at

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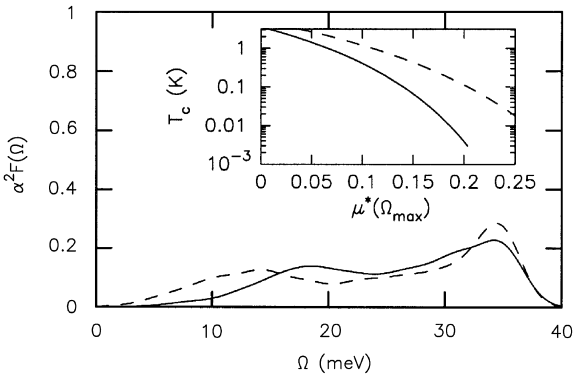

Fig. 1 . Electron–phonon spectral function for Li in the 9R and BCC phases. The superconducting T_c is plotted on a semilog plot versus $\mu^*(\Omega_{max})$ in the inset. The solid lines are for the 9R structure and the dashed for BCC.

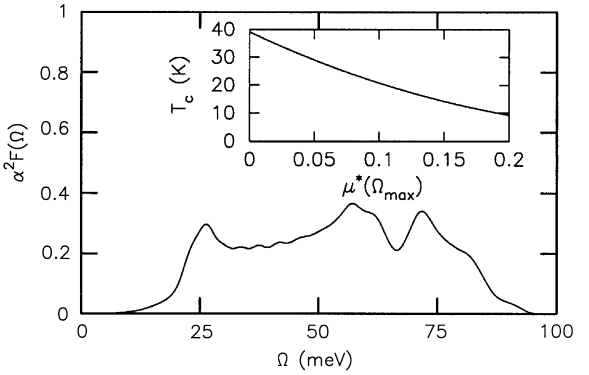

Fig. 2. Electron–phonon spectral function of S at 200 GPa in the β-Po phase. The superconducting T_c is plotted versus $\mu^*(\Omega_{max})$ in the inset.

160 GPa. We report here on the coupling of electrons to phonons in this β-Po phase at 200 GPa.

Fig. 2 plots α^2F versus Ω and plots T_c versus $\mu^*(\Omega_{max})$ in the inset. The electron–phonon coupling strength is only $\lambda = 0.77$, but the T_c is so large because of the high-frequency phonons (the upper cutoff lies near 95 meV). We find that $\mu^* = 0.125$ is the right size to produce the observed values of T_c. The theoretical calculations can be used to predict other superconducting properties, including the tunneling conductance, which is difficult to measure under pressure.

4. Conclusions

Theoretical calculations of superconductivity have reached the point where they are competitive with experi mental techniques for real materials. In Li electrons couple more weakly to phonons in the 9R phase than in the BCC phase, explaining a low value of T_c, and in high-pressure S the high T_c arises from the large phonon frequencies.

Acknowledgements

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