Abstract

Calculations of the electron-phonon interaction in the alkali metals, Potassium and Rubidium, using the results of band theory and BCS theory-based techniques suggest that at high pressures K and Rb would be superconductors with transition temperatures approaching 10K.

Key words: A. superconductors, D. electronic band structure
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In a recent paper Shimizu et al.[1] reported the discovery of superconductivity in compressed Lithium with a transition temperature $T_c = 20K$. This report is a confirmation of previous theoretical work of Neaton and Ashcroft,[2] who predicted that at high pressures Lithium forms a paired ground state, and of Christensen and Novikov,[3] who suggested that fcc Lithium under increased pressure may reach $T_c = 50-70K$.

In this work we applied a methodology similar to that of Ref.[3] to the alkali metals K and Rb. The procedure goes as follows: we first performed Augmented Plane Wave (APW) calculations of the band structure and total energy of the above alkali metals in both the bcc and fcc structures over a wide range of volumes reaching high pressures. From these calculations we obtained...
Fig. 1. Angular Momentum decomposed DOS divided by total DOS at \( \varepsilon_F \) the Fermi level, \( \varepsilon_F \), values of the density of states, \( N_t \), and its angular momentum decomposition, \( N_l \), as a function of volume. We also used the APW results to determine the volume variation of the bulk modulus \( B \). We then used the self-consistent APW potentials to determine the scattering phase shifts \( \delta_l \) again as a function of volume. The quantities \( N_l \) and \( \delta_l \) were then used in the “rigid muffin-tin” approximation[4,5] to determine the Hopfield parameter \( \eta \).

The next step was to calculate the electron-phonon interaction parameter,

\[
\lambda = \frac{\eta}{M <\omega^2>}.
\]  

We accomplished this by assuming[6] that

\[
<\omega^2> = CBV^{1/3},
\]

where the constant of proportionality C was determined from from the experimental values of \( B \), \( V \) and the Debye temperature \( \theta_D \).

In Fig. 1 we show the ratios \( N_l(\varepsilon_F)/N_l(\varepsilon_F) \) at the Fermi level \( \varepsilon_F \) as a function of volume. These ratios are crucial in the determination of \( \eta \). It is important to note that the ratio \( N_d(\varepsilon_F)/N_l(\varepsilon_F) \) increases rapidly as we go to smaller volumes. This build up of the d-like DOS under pressure causes the large values of \( \eta \) at small volumes shown in Fig. 2.

In this theory there are three contributions to \( \eta \) coming from the channels s-p, p-d and d-f. The d-f contribution is negligible but the p-d contribution is comparable to the s-p at large volumes and becomes larger at small volumes.
where superconductivity occurs. Also in Fig. 2, we show the variation with volume of the denominator of (1), $M <\omega^2>$, which we have extracted from the variation of the bulk modulus.

In Fig. 3, we show the electron-phonon coupling $\lambda$ as a function of volume determined from (1). It is evident that at small volumes $\lambda$ reaches large values suggesting that these metals can display superconductivity under pressure. To quantify our prediction for superconductivity on the basis of strong electron-
phonon coupling, we have calculated $T_c$ using the McMillan equation[7,8] with a Coulomb pseudopotential value $\mu^* = 0.13$. These results are also shown in Fig. 3.

It is clear that transition temperatures in a range of 5-10 K are reachable for both the fcc and bcc lattices at volumes in the neighborhood of $V/V_0 \approx 0.4$. We have calculated that such volumes correspond to pressures of 13.5 GPa for K and 8 GPa for Rb, respectively.

The similarity of our fcc and bcc results suggests that our prediction of superconductivity in K and Rb is independent of crystal structure. We believe that our prediction is still valid even if, experimentally, these materials under high pressure transform to other structures such as $hR1$ or $cI16$. We propose that the mechanism of superconductivity in these metals is due to the increased d-like character of the wave-functions at $\varepsilon_F$ at high pressures, which validates our use of the “Rigid Muffin-tin” approximation that is successful in transition metals.

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