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A. van Kessel, H. Myron, F. Mueller. HIGH PRECISION BAND CALCULATION OF Nb₃Sn
IN THE A-15 CUBIC PHASE. Journal de Physique Colloques, 1978, 39 (C6), pp.C6-414-C6-415.
10.1051/jphyscol:19786186 . jpa-00217601

HAL Id: jpa-00217601

<https://hal.science/jpa-00217601>

Submitted on 1 Jan 1978

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HIGH PRECISION BAND CALCULATION OF Nb_3Sn IN THE A-15 CUBIC PHASE

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Résumé.- Un nouveau calcul de haute précision a été effectué pour les bandes de Nb_3Sn au moyen de la méthode APW; des corrections au potentiel y sont incluses et à l'intérieur et à l'extérieur de la sphère muffin-tin. Les résultats (surface de Fermi, densité d'états, etc..) sont en bon accord avec huit expériences différentes. Nous en concluons que notre modèle est d'une bonne précision.

Abstract.- A new precision band calculation has been undertaken for Nb_3Sn using the APW method with potential corrections included inside and outside the muffin-tin spheres. The results (Fermi surface, density of states, etc..) show good agreement with eight experiments. It is concluded that the band model is highly accurate.

Interest in the A-15 high temperature superconductor Nb_3Sn began with its discovery over 20 years ago /1/, yet interest remains high today. Primarily this recent interest focused on a number of anomalous normal state properties /2/, those measured above the superconducting transition temperature. Theoretical models have been used to correlate or make these anomalous properties understandable. Many of these have focused on the explicit point group symmetry of selected points in the Brillouin zone; others have invoked the use of tight-binding schemes with a variety of couplings within or between the dominant d-electron Nb-chains. In this paper we treat the electronic structure globally /3/. Our technique and methodology is similar to the well known APW work of Mattheiss /4/. We differ in only two ways : i) the inclusion of non-spherical potential corrections within the muffin-tin spheres; ii) the use of the APW secular matrix itself as an "interpolation scheme", without reliance on an intermediate Slater-Koster like fit, when extreme precision was desired. All elements were treated so as to maintain an overall precision of better than 3 mRy. The details will be published elsewhere /3/. Both Mattheiss and ourselves fit the XPS spectra /5/ equally well.

In Figure 1 we show the band structure on a fine scale. Making a microscopic comparison with Mattheiss' Figure 6(d), one can see that there are major changes. The bands associated with Γ_{12} have become flatter and an entire set of bands near M has "popped up" through the Fermi level (E_F).

Fig. 1 : The band structure of Nb_3Sn near E_F .

Raising E_F by 2 electrons/unit cell, we find intersections which agree well with the Nb_3Sb dHVA structure of Reference /6/. Since most of the electrons near E_F in both Nb_3Sn and Nb_3Sb are primarily due to Nb d-electrons such "rigid band" behavior is not really surprising. Nevertheless, a careful examination shows that a rigid band model has even quantitative accuracy.

In Figure 2 we show the density of states, $N(E)$, on a similar scale as Figure 1. The values shown were linearly interpolated between a sequence of values of energy spaced 1.25 mRy apart. Although it is always possible that fine structure in $N(E)$ of A-15 materials exists "between" the grid we have chosen, we believe that the probability for such fine structure falling just at E_F is unlikely. Thus in our results the peaks in $N(E)$ are narrow compared with that for a typical transition metal.

Fig. 2 : The density of states near E_F .

The Γ_{12} levels in Figure 3 are about 20 mRy wide compared with 150 mRy for a typical transition metal, but our narrow peaks are vastly broader than a typical thermal energy $k_B T$ - about 2 mRy for 300 K. We find no evidence to support a Jahn-Teller effect.

Using the value of $N(E_F)$ we find consistent behavior with both the electronic part of the specific heat /7/ and the temperature dependence of the susceptibility /8/, details will be published elsewhere /3/.

In figure 3 we present the derived Fermi surface of Nb_3Sn . The results are rather complicated reflecting the eight atom/unit cell geometry in real space. Yet two simplifying features emerge: i) the set of light mass oscillated ellipsoids centered at M; ii) the flat box-like structures centered at Γ . Recently dHVA /9/ oscillations have been seen consistent with the M centered structure. Positron annihilation measurements /10/ in the (100) direction of isoelectronic V_3Si show structure at 0.185, 0.635 and 0.844 π/a units.

Fig. 3 : The Fermi surface of Nb_3Sn .

The calculated intersection of the Fermi surface "flat" sheets along Γ to X are 0.15 and 0.64 π/a units, in good agreement with the first two pieces of structure. The twentieth band near X along with the 20th band surrounding the X-R line is a possible candidate for the third structure but this identification is tentative. We have also assumed a microscopic similarity between the electronic structure of Nb_3Sn and V_3Si in the above.

In summary the electronic band structure we have calculated fits globally as seen for the comparison with the XPS work /5/, fits in zeroth derivative of $N(E)$ at E_F /7/, fits in the first derivative as seen from the temperature dependence of the susceptibility /8/, fits the Hall constant /11/, fits the Junod value of the electronic specific heat /7/, fits the dHVA data of Nb_3Sb in the rigid band sense /6/ as well as Nb_3Sn /9/, and fits some of the β^+V_3Si data /10/. We know of no previous A-15 calculation which has simultaneously fit so many experiments.

This work was performed as part of the research program of the "Stichting voor Fundamenteel Onderzoek der Materie" (FOM) with financial support from the "Nederlandse Organisatie voor Zuiver Wetenschappelijk Onderzoek" (ZWO).

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