ELECTRONIC STRUCTURE, ELECTRON-PHONON INTERACTIONS AND LOW-TEMPERATURE ANOMALIES IN A15 COMPOUNDS

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Résumé.- En nous servant de nos calculs ab initio de la structure de bande par la méthode APW self-consistante, nous discutons la structure fine dans la densité des états électroniques près du niveau de Fermi, et l'interaction électron-phonon pour les composés A15 v_3X et Nb_3X, avec X = Al, Ga, Si, Ge et Sn.

Abstract.- Using our ab initio self-consistent APW band calculations, we discuss fine structure in the electronic density of states near the Fermi level, and the electron-phonon interactions for the A15 compounds v_3X and Nb_3X, with X = Al, Ga, Si, Ge and Sn.

Theoretical work on the A15 materials has centered on relating the low-temperature anomalies and the high values of T_c in many of these compounds /1/. Following the work of Clogston and Jaccarino /2/ who postulated the existence of a sharply peaked electronic density of states (DOS) near the Fermi energy (E_F), there have been several models of the band structure /3-7/ which have yielded such peaks. Most of these models make use of the quasi-one-dimensionality of the A15 structure. Several ab initio band structure calculations have been done for A15 materials /8-10/ which have not verified the underlying assumptions of the model calculations, but they have lacked sufficient accuracy to study the fine structure in the DOS near E_F.

More recently /11/ we have done highly accurate APW calculations for ten different A15 compounds : v_3X and Nb_3X, with X = Al, Ga, Si, Ge and Sn, covering the range of high and low-T_c. The purpose of this work is to examine the Fermi surfaces and related properties of these compounds in some detail. The techniques used, self-consistency, relativistic, warped muffin-tins,etc..., are fully described elsewhere /11/. Here we will discuss some aspects of these results, namely the electron-phonon interactions (e-p-i) and sharp DOS structure of these materials.

Figure 1 shows the DOS near E_F for two A15 compounds, Nb_3Sn and V_3Ge respectively, in a very narrow energy range $\pm$ 3 mRy (1 mRy $\sim$ 150 K). It is clear from figure 1 that Nb_3Sn which has rather drastic low-temperature electronic properties (contrary to V_3Ge) also has a very rapid DOS variation near E_F, while the behavior of the DOS (N) of V_3Ge is nearly constant in the range $\pm$ 300 K, around E_F.

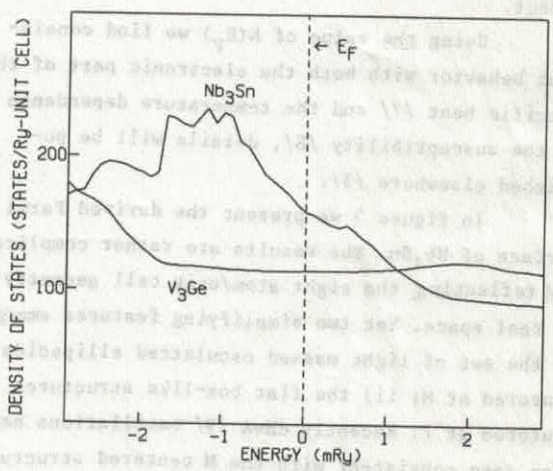

Fig. 1 : Electronic density of states near E_F for Nb_3Sn and V_3Ge.

The behavior of Nb_3Sn, $(\Delta N/N)E_F$ is of order unity in a range $\Delta E \lesssim 100$ K, is of the right magnitude to explain the observed anomalous low-temperature behavior. Our calculations also show that results similar to Nb_3Sn arise for V_3Si, V_3Ga, and to a somewhat lesser extent for Nb_3Al and Nb_3Ga /11/. On the other hand the relatively "normal" materials (e.g. V_3Al and V_3Sn) behave similarly to V_3Ge. We should emphasize two additional points : 1) the DOS fine structure arises from a fully ab initio APW calculation; and 2) the unusually flat bands giving rise to the DOS fine structure comes

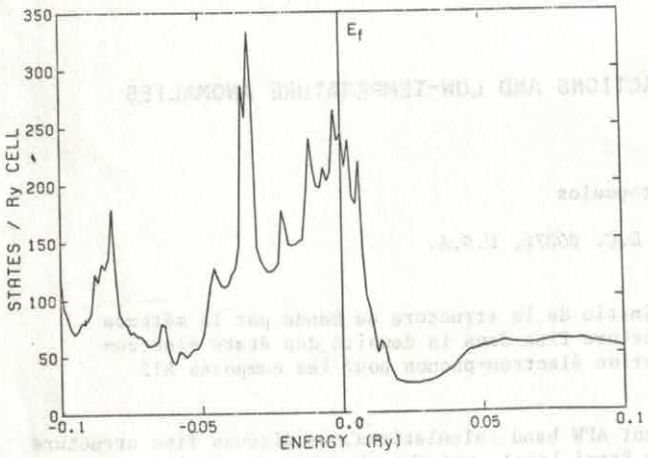

Fig. 2 : The density of states near E_F.

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_BT - 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 massed osculatted 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, o.635 and 0.844 π/a units.

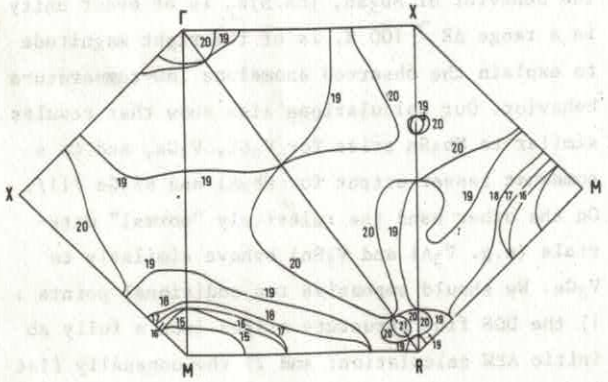

Fig. 3 : The Fermi surface of Nb_3Sn.

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.

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