

TABLE III. Energies in electron volts.

	$ V_{110} $	V_{110} (Ham)	Δ_{110}
Li	1.3	1.37	1.3×10^{-2}
Na	0.18	0.11	5×10^{-4}
Cs	0.50	-0.57	2×10^{-2}

equal in this approximation to the specific-heat mass.¹⁷ The agreement between the calculated and experimental masses is reasonable and indicates the need for further data on the remaining alkali metals.

Fermi-surface mapping for Li, Na, and Cs is as yet very incomplete. In the case of Li and Na complications arise through the tendency of these metals to undergo a martensitic transformation into the hcp phase at low temperatures. Some indication of the size of the first band gap in these metals may be obtained by using the specific-heat effective masses and working back through the corresponding β 's. These are marked with an "a" in Table II. Ignoring contributions from V_{200} for the moment we find values for $|V_{110}|$ as listed in Table III. We have compared them with Ham's calculated values and the agreement is satisfactory. The distortions along the [110] direction can be evaluated with the aid of (6) and they are listed in Table III. In Li some comparison may be made with dimension obtained from position annihilation experiments.¹⁸ These give a dimension

¹⁷ S. Nakajima and M. Watabe, *Progr. Theor. Phys. (Kyoto)* 30, 772 (1963).

¹⁸ J. J. Donaghy, A. T. Stewart, J. H. Kusmiss, and D. M. Rock-

corresponding to $\Delta_{110} \sim 0.03$, in some disagreement with our figure but confirming as we do that there is likely to be no contact of the Fermi surface with the nearest zone boundary (assuming we are dealing with the bcc phase). Shoenberg and Stiles are able to give an upper limit on the distortions to the Fermi surface in sodium of about 5×10^{-4} , in good agreement with our rough figure. There is no data of sufficient accuracy in Cs with which to compare the dimension obtained here. The effect of including a set of (200) planes does not alter significantly the value of the V_{110} band gap. For example, in Rb the ratio V_{200}/V_{111} has the value 3.3. If we use the same ratio in Cs the effect is merely to lower V_{110} to 0.42 eV.

Finally, using the band gaps and parameters listed in Tables I-III we may readily determine the Fermi energy (as measured from the band minimum) and hence evaluate the minimum energies required for direct and indirect (e.g., phonon assisted) interband transitions. In K and Rb these are 1.43, 0.89 and 1.16, 0.99 eV respectively. Using the estimates of the band gaps given in Table III the corresponding values for the metals Li, Na and Cs are 5.3, 4.3; 2.05, 1.14; and 1.64, 1.36 eV respectively.

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