Electron-Phonon Interactions in Solid Alkali Metals. I. Scattering and Transport Coefficients*

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In an earlier article,[1] room-temperature electronic transport coefficients were calculated for all the solid alkalis using a phonon structure factor given by the simplest Born–von Karman dynamical matrix compatible with and fixed by the elastic constants. The values so calculated were found, for Na and K, to agree within 1 to 10% with those obtained using accurate structure factors (see Table IV of Ref. 1). Since the completion of our calculations, neutron inelastic scattering results and Born–von Karman fits to phonon dispersion curves have been reported also for Li[2] and Rb,[3] and we have now repeated all calculations for Li and Rb using accurate structure factors. No neutron data for Cs are yet available.

In Table I these new results are listed and compared to those previously reported (notation is as in Ref. 1). Again, we find no differences significant at presently attainable levels of accuracy in microscopic transport theory. This is particularly noteworthy in the case of Li, where there is evidence in the LA modes of long-range forces,[2] and where, moreover, an error of almost 50% in the thermopower coefficients can be produced by a 5% error in the quantity actually calculated numerically (namely, the electron mean-free-path integrand and integral). These results indicate that the simple elastic-constants dynamical matrix can be used without presently significant sacrifice of accuracy, in calculation of ordinary electronic properties of the bcc solid alkali metals.

TABLE I. Thermopower coefficients ξ_k, resistivities r_k ($\mu\Omega$ cm), mean free paths l_k (Å), and effective number of charge carriers per electron (n^*/n). Comparison of values calculated using phonon structure factors in the elastic-constants approximation (*E*) and obtained from neutron inelastic scattering data (*N*). For details and experimental values see Ref. 1.

	Li		Rb	
	E	*N*	*E*	*N*
ξ_{100}	−1.89	−2.34	2.93	2.93
ξ_{110}	−6.24	−6.45	2.63	2.63
ξ_{111}	−3.02	−3.97	2.74	2.74
ξ_{av}	−3.49	−3.89	2.73	2.74
r_{100}	6.77	5.95	2.22	2.04
r_{110}	20.33	20.02	2.29	2.11
r_{111}	18.50	19.61	2.24	2.08
r_{av}	13.62	12.90	2.26	2.08
l_{100}	145.5	165.6	1133.0	1234.3
l_{110}	48.5	49.2	1100.0	1191.3
l_{111}	53.3	50.3	1120.7	1210.4
l_{av}	72.3	76.4	1114.0	1207.1
n^*/n	0.76	0.71	1.000	1.000

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