Pressure dependence of phonon dispersion curves in simple metals†

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Abstract. The reliability of different forms for the bare electron–ion model pseudopotential and for the dielectric screening function has been studied by calculating, at variable volume, phonon dispersion curves in the simple metals sodium, aluminium and lead. We find that inclusion of exchange and correlation effect in the dielectric function is essential for agreement with experiment, and that the precise form of the corrections for these is also very important. Shaw's optimized non-local potential, when suitably screened, yields good agreement with experiment at zero pressure for sodium and aluminium, and better agreement than is obtained with the local version of the Heine–Abarenkov potential. Pressure derivatives of the elastic constants for these metals, as predicted from the Heine–Abarenkov potential, are reasonably accurate, while the pressure derivatives of the maximum phonon frequencies yield good qualitative agreement with the experimental pressure derivative of the superconducting transition temperature in aluminium. For lead, the agreement with experiment of the dispersion curves and pressure derivatives is generally poor.

1. Introduction

Before meaningful theoretical studies of complex properties of metals, such as the electron–phonon interaction and superconducting transition temperatures, can be made, the reliability of the model potential or pseudopotential used to represent the electron–ion interaction must be known. In this paper we have used calculations of the phonon dispersion curves and their pressure derivatives to study these potentials for the simple metals sodium, aluminium and lead.

Estimates of the potential at the first few reciprocal lattice vectors can be obtained from fits to the Fermi surface as determined via de Haas–van Alphen experiments, but this is not sufficient to verify the accuracy of the potential at all values of momentum transfer. However, calculated phonon frequencies depend on the entire potential, so comparison of these with experiment provides a much more refined method of testing the various potentials suggested by different authors. Calculations at decreased volume permit a further check.

Many calculations of phonon dispersion curves in simple metals have been performed in recent years, using a variety of such electron–ion potentials. For instance, Vosko *et al.* (1965) used a single orthogonal plane wave approach for a non-local pseudopotential to calculate dispersion curves in Na, Al and Pb; Animalu *et al.* (1966) used a local Heine–Abarenkov (1964) model potential in calculations for the alkali metals and Al; and Shaw and Pynn (1969) used Shaw's (1968) optimized non-local model potential in a calculation for Mg. Calculations of the elastic constants have been performed by, among others, Shyu and Gaspari (1969), who used Ashcroft's (1966) local model potential for the alkali metals and Al.

Nearly all the calculations for the alkali metals agree well with the dispersion curves obtained from inelastic neutron scattering experiments. This is mainly because the conduction electron response to the vibrating ions, through which the pseudopotential enters the calculation, accounts for a relatively small proportion of the effective interaction between

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