LATTICE DYNAMICS, NEUTRON SCATTERING AND BAND STRUCTURE OF ONE- AND TWO-DIMENSIONAL LATTICES

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PREFACE

The present thesis is a study of lattice dynamics, neutron scattering and band structure of linear and layer lattices. It consists of five chapters.

In Chapter I, which is the introduction to the thesis, we have discussed the reasons for choosing one- and two-dimensional structures for the present study. A brief outline of the work presented in other chapters is given and a review of the previous work done is also given.

In Chapter II, we have discussed the lattice dynamics of infinite linear and layer lattices. We have discussed the effect of including angular forces on the vibrational properties of one- and two- dimensional lattices. In two-dimensions we have considered the dynamics of a square lattice and of a hexagonal lattice. The latter study has been applied to the graphite lattice. The results of this chapter have been reported in the following paper:-

"Transverse Vibrations of Linear and Layer Lattices", American Journal of Physics, 39 (1971) 166.

In Chapter III, we have carried out an exact normal mode analysis for a diatomic linear lattice, with a defect atom at the centre, taking free end boundary conditions. The force constants associated with the defect atom as well as the surface atoms have been taken to be different than the bulk value. Local modes for H^- centre in NaCl, NaBr and KCl lattices have been calculated. The results of this

chapter are published in the following two papers:

1. "Local and Gap Modes due to a Substitutional Impurity in Alkali Halides: One-dimensional Treatment", Physics Letters, 39A (1972) 179.

2. "Local and Gap Modes due to Surface or Substitutional Impurity in Diatomic Linear Lattices" Journal of Physics and Chemistry of Solids, 33 (1972) 1885.

In Chapter IV, the existence of surface modes is investigated in a monatomic linear lattice with free ends and having alternate atomic spacings. The results of this chapter are presented in the following paper:

"Extension of Louck's Method for Calculating Normal Modes for Finite Lattices", Accepted for publication in Physica.

In Chapter V, we have discussed a procedure for evaluating the scattering cross sections for linear and layer lattices. The results of this chapter are published in the following paper:

"Neutron Scattering from One- and Two-dimensional Structures", Journal of Nuclear Energy, 26(1972) 409.

In Appendix-A, we have discussed the effect of size on the band structure of a finite one-dimensional lattice. The results of this chapter are published in the following short note:

"Effect of Size on the Band Structure of a Finite One-dimensional Lattice", Physica Status Solidi (b), 48 (1971) K173.

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