AEC-NASA TECH BRIEF

Study of Lattice Defect Vibration

The report presents the notes from a series of five lectures on the vibrations of defects in crystals, given by Dr. R. J. Elliott of the Department of Theoretical Physics, Oxford, England. The lectures concern many theoretical ideas current in research on vibrations in imperfect crystals. Principally they relate the classical Green's-function techniques to the more modern thermodynamic Green's-functions methods.

These lectures concern the manner in which defects, well localized in a crystal but interacting strongly with the other atoms, change the properties of a perfect crystal. The basis of the mathematical methods used to treat this problem is quite general and is the same as that used to calculate changes in the electronic or magnetic properties of a defected crystal. All the methods typically used to solve defect problems can be called Green's-function methods; they relate the properties of an imperfect lattice to the properties of a perfect lattice.

The five lectures given by Dr. R. J. Elliott are as follows:

I. Perfect and Imperfect Crystals and Green's-Function. This section develops a technique by which the normal modes of vibration (and their frequencies) can be found for a crystal having a single localized imperfection.

II. Solutions of the Perturbed Dynamical Matrix; Electron and Magnon Analogies. This section uses the technique developed in Section I to determine the normal vibrational modes and frequencies of a crystal with a single defect. A detrimental resonance condition is found for localized modes, at a frequency above the maximum frequency of the perfect-crystal modes, and for "in-band" modes, which cover the entire crystal with possible enhancement near the defect.

III. Response of a System to a Force and Double-Time Green's-Functions. This section relates the Green's-functions to their spectral representations and to the correlation function of two canonical particle coordinates at different times and places. A harmonic quantum-mechanical equation of motion for the displacement Green's-function is solved.

IV. Physical Results From a Double-Time Green's-Function Treatment. This section demonstrates the ease with which the thermal Green's-functions may be used to calculate observable physical quantities.

V. Physically More Realistic Models. A number of interesting effects due to a harmonic coupling of a light defect atom to the host crystal are discussed.

Notes:

1. Additional information may be found in the report, "Vibrations of Defects in Lattices," ANL-7237, Argonne National Laboratory, July 1966. This report is available from the Clearinghouse for Federal Scientific and Technical Information, Springfield, Va. 22151; price: $3.00 each (microfiche copies, $0.65 ea.), Reference: B69-10078.
2. The study contributes to the basic understanding of aspects of crystal vibrations. Because of the wide use of crystals in industry, this work is significant since it summarizes and unifies much previous theoretical work on the effects of crystal defects.
3. Inquiries concerning this innovation may be directed to: Office of Industrial Cooperation
   Argonne National Laboratory
   9700 South Cass Avenue
   Argonne, Illinois 60439
   Reference: B69-10078

Source: R. J. Elliott
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(ARG-10221)

(continued overleaf)

Patent status:

Inquiries about obtaining rights for commercial use of this innovation may be made to:

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