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Autor: Szigeti, B.
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On impurity effects in the infra-red and at ultra-high radio frequencies in solids

(Summary of paper to be presented at the Ampere Conference at Pisa, September, 1960).

by B. Szigeti

Department of Theoretical Physics, University of Liverpool

In recent years a number of papers dealt with various impurity effects connected with the vibrations of solids. Some of these are summarized in the review articles by Lifšic (1956) and Montroll et al. (1958). The present paper describes the first stage of a theoretical investigation on the effect of small amounts of impurities on the vibrational absorption spectrum of unpolar crystals. This is of interest, for instance, in connection with diamond, silicon and germanium. In the presence of small amounts of impurities (less than 1%) these materials exhibit characteristic absorption in the region of the lattice frequencies while in the pure state they show no absorption in that region. The results obtained, however, are not limited to these materials but are of interest in connection with all types of vibrational absorption due to impurities in solids. This type of absorption is usually in the infra-red, but in some cases it is at ultra-high radio frequencies.

At the first stage of this investigation, using the results of a previous paper by the author (1952), exact solutions have been obtained for the absorption due to a single impurity atom in a linear chain of uncharged atoms. It is found that the impurity atom takes part in almost all the modes of vibration of the chain, and to a larger or smaller degree, makes them all active in the absorption spectrum. The quantitative solution shows that the absorption due to this effect has a well pronounced maximum at a frequency which depends upon the nature of the impurity but is always lower than ν_{max} the highest vibrational frequency of the chain.

Under certain conditions, if mass and force constant of the impurity atom are favourable, there is also a further absorption line at a frequency

higher than ν_{max}. This line arises from a vibration where only the impurity atom and its immediate neighbours vibrate.

The result allows certain conclusions concerning impurity effects in a 3-dimensional solid. It also indicates that by the admixture of impurities it is possible to make such modes of vibration appear in the absorption which, in the pure state, are not active either in the absorption or in the Raman spectrum.

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DISCUSSION

M. Palma. — I should like to ask wether a temperature-dependence, down to a few absolute degrees, of the impurities spectrum is expected and (if this is the case) if it might be related to anharmonic phonon- scattering processes by impurities.

M. Szigeti. — The impurities are bound in the lattice essentially by harmonic forces; hence their most important effect is to alter the harmonic part of the lattice vibrations, and the absorption due to this effect should be independent of temperature.