shapes and magnitudes of these curves can be made. Since the electrical resistivity of both crystals was greater than 10^5 ohm cm at all temperatures, only the lattice conductivity should be important. The magnitude of the thermal conductivity at the Debye temperature, K_θ, can be estimated.[2] A value of $\gamma = 2$ is assumed for the Grüneisen constant of both materials, and a Debye temperature of 410°K is used[3] for NiO and 230°K for[4] MnO. This gives $K_\theta = 0.19$ watt/cm deg for NiO and 0.059 watt/cm deg for MnO. As seen from the graph, the order of magnitude agreement is satisfactory. The K_θ values are calculated assuming that Umklapp-processes are the only mechanism producing thermal resistance. This is clearly not the case in MnO where there is a decided minimum in the thermal conductivity curve at the Néel temperature (120°K) at which MnO changes from an antiferromagnetic state to a paramagnetic one. The lattice distortion[5] which occurs at the Néel point seems to be too small to explain this effect. In addition to the Umklapp scattering, it appears that there is an additional interaction between the phonons and the magnetic moments of the manganese atoms which serves to scatter the phonons. A similar minimum in the thermal conductivity of single crystals of NiO might also be found at its Néel temperature (525°K). Earlier investigations[6] on compressed powder samples of NiO failed to exhibit such a minimum.

Since the thermal conductivity is proportional to the specific heat, one might expect to find a λ-type anomaly in the thermal conductivity similar to that found[4] in the specific heat at the Néel temperature. Although such an anomaly was looked for very carefully during the thermal conductivity measurements, none was found. This indicates that the thermal conductivity associated with the magnetic ordering anomaly in the specific heat curve is less than a few percent of the lattice thermal conductivity at the Néel point.

The thermal conductivity of a perfect insulating crystal at low temperatures should be determined by boundary scattering[7] of the phonons. The magnitude of the boundary scattering has been estimated using the sample diameter, the Debye temperature, and the average sound velocity calculated from the Debye temperature. For NiO with an average velocity of 2.9×10^5 cm/sec the result is $K = 0.11\, T^3$ watt/cm deg[4]. The observed K at the lowest temperatures varies as T^3, but is a factor of 140 less than the calculated value. This indicates an equivalent mean free path for the phonons of 30 microns. For MnO the average velocity is 1.7×10^5 cm/sec, which gives $K = 0.34\, T^3$ watt/cm deg[4]. Since the observed K is nearly proportional to T^3, the data indicates a mean free path of 0.5 microns. Thus the external boundaries are not limiting the thermal conductivity at low temperatures; some other scattering mechanism is required to explain the results. This may be the interaction with strains, precipitates, spin waves, or antiferromagnetic domain walls. Further experiments using annealed crystals and crystals grown by other techniques are underway in an attempt to clarify the problem.

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LATTICE VIBRATIONAL SPECTRA OF Si AND Ge

H. Cole and E. Kineke
International Business Machines
Research Laboratory,
Poughkeepsie, New York

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There are two basic ways at the moment for obtaining the lattice vibrational spectrum of a crystal if one has the experimentally determined dispersion relations for the elastic waves traveling in certain directions in the crystal. One is based on an interpolation method which reconstructs the whole vibrational spectrum from the behavior of the dispersion curves at certain singular points in the Brillouin zone[1-3]; the

other uses a brute-force machine calculation based on analyzing the dispersion curves to obtain a set of interatomic force constants and then calculating enough of the remaining frequencies to sample the distribution adequately.[4]

A program, based on the Born-von Kármán theory of lattice vibrations, has been written for an IBM 704 in order to carry out the latter procedure. With the interatomic force constants as input, the program will generate the elements of and solve the Hermitian matrices for several thousand wave vectors for certain cubic crystals, including forces out to sixth-neighbor, and print out all or any of the frequencies and polarization vectors and/or the frequency distribution. As there is special interest in the vibrational spectra of Si and Ge, and since sets of interatomic force constants are available, these spectra as computed with this program are reported on below.

Figure 1 is the vibrational spectrum of Ge obtained by using a set of force constants derived from the dispersion curves of waves traveling in the [100] and [111] directions. The dispersion curves were obtained by Brockhouse using neutron scattering.[5] The set of force constants used were derived by Herman[6] and, independently, by the authors. It was found necessary to include forces out to sixth-neighbor. Herman reported several possible sets; some were ruled out by him on physical grounds and by the authors since the sets predicted imaginary frequencies along the [110] axis and in other directions. However, Herman's remaining sets gave essentially the same distribution although they

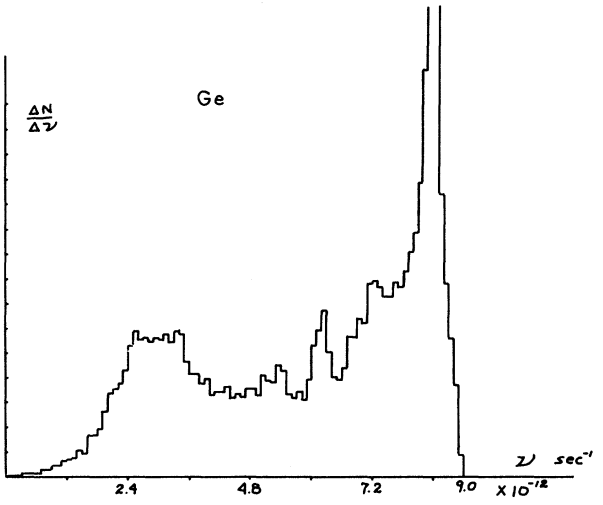

FIG. 1. Lattice vibrational spectrum of Ge.

predicted different [110] dispersion relations. Further experimental results are needed to define properly a unique set. The fact that sixth-neighbor forces play a role is somewhat surprising. Attempts to explain certain aspects of the forces in Ge have been made by Lax.[7]

Figure 2 is the vibrational spectrum of Si obtained by using a set of force constants derived by Learn[8] from x-ray scattering experiments.

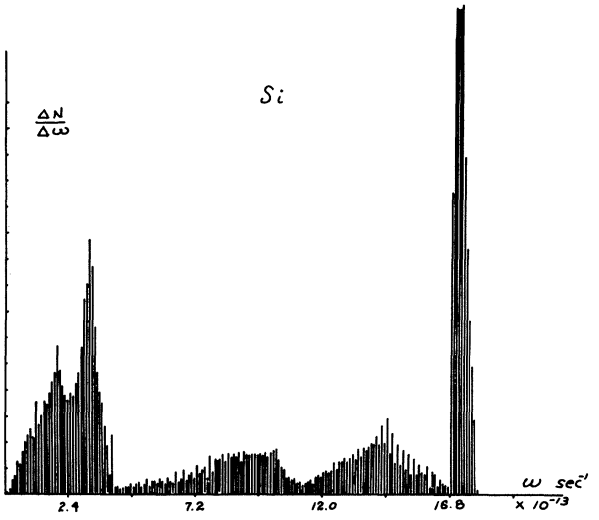

FIG. 2. Lattice vibrational spectrum of Si.

These constants assume that all forces beyond third-neighbor are negligible, and, as in the case of Ge, the antisymmetric second-neighbor constant was taken to be zero. In view of the fact that the convergence properties of the force-constant model with respect to the addition of further neighbors have not been explored, these spectra should be treated as somewhat tentative. Earlier calculations were made by Hsieh[9] using even simpler sets of constants.

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