Bull. Amer. Phys. Soc., 15, 1623 (1970)

EE 3. Raman Spectra of Single Crystal Hydrogen and Deuterium in the Ordered State. W. N. HARDY and I. F. SILVERA, Science Center, North American Rockwell Corp., and J. P. McTAGUE, Univ. of Calif., Los Angeles--We have grown large (~ 1 cm^3) single crystals of high purity (~ 98%) ortho-hydrogen and para-deuterium and obtained the Raman spectra in the orientationally ordered state. The intensities, polarization properties, and frequencies have been measured for the librons, rotons, and the J=0→2 impurity transitions. The frequency shifts have been determined to better than 0.1 cm^{-1}. Doubt cast upon the assignment of the space group Pa3 to the structure of the ordered state by previous Raman results[1] has now been removed. Good agreement is obtained between experimentally observed and theoretically calculated intensities if the three lowest frequency modes are assigned to the E_g, T_g^1 and T_g^2 modes of the Pa3 structure. The broad feature previously observed[1] at higher frequencies is assigned to a two-libron scattering process.

[1]I. F. Silvera, W. N. Hardy, and J. P. McTague, Disc. of Faraday Soc. 48, 54 (1969).

EE 4. Raman Spectrum of KTN.* S. K. MANLIEF and H. Y. FAN, Purdue Univ.-- Raman scattering from the mixed crystal $KTa_{.65}Nb_{.35}O_3$ (T_c = 10°C) has been investigated as a function of temperature in the paraelectric and single domain ferroelectric phases. The second order structure did not change significantly over the temperature range studied while the first order scattering disappeared abruptly as the crystal was heated above the transition temperature, as required by symmetry. A wing of E mode symmetry extending out from the laser line was observed whose intensity decreased with increasing temperature and disappeared in the paraelectric phase. This appears to be the overdamped soft mode. Two peaks, one of A_1 mode symmetry and one of E mode symmetry, were observed whose frequencies decreased monotonically as the temperature was increased toward T_c. A peak observed at 279 cm^{-1} is assigned to the silent mode. Other first order peaks were observed at 204, 419, 550, and 825 cm^{-1}. In addition, first order lines were observed with symmetry properties forbidden for an ideal perovskite structure.

*Work supported by Army Research Office (Durham) and Xerox Corporation.

EE 5. Raman Scattering in a Linear Crystal Lattice with "Periodic Impurities". S. M. LEE, R. A. MANN, and J. A. LEU, Mich. Tech. Univ.--Raman intensity is calculated for a semi-infinite monatomic linear lattice which is modified by substitutional isotopic impurities at alternating lattice sites. Only the nearest-neighbor harmonic interaction forces are considered. The calculation is based on a recently obtained vibrational analysis for the lattice model[1] which simplifies the analysis. The Raman intensity is proportional to $R(\omega_r) \sim [1-(-1)^r]^2 |\partial\alpha/\partial(\Delta u)|^2 \cos^2(k_r \xi/2)$, where $\partial\alpha/\partial(\Delta u)$ is the change of polarizability with respect to the relative displacements of nearest neighbors and $k_r = r\pi/N\xi$ for the system containing N atoms at ξ apart. The factor $[1-(-1)^r]$ shows that only the odd modes are Raman active. The result is similar to the expression for the Raman intensity for a monatomic chain[2], showing that the effect of the impurities is very small in the semi-infinite limit. The lattice model treated here is equivalent to a diatomic linear lattice. Thus the calculation facilitates a simple means of approximation for the usually complicated problem dealing with the diatomic model.

[1]S. M. Lee, Am. J. Phys. 37, 888 (1967).
[2]M. Hass and H.B. Rosenstock, Appl. Opt. 6, 2079 (1967).

EE 6. Pressure Dependence of Vibrational Infrared Absorptions of Polymorphisms of Silica.* K.CHOW and A.I.BIENENSTOCK, Stanford University.--The pressure-induced frequency shifts of the infrared-active lattice vibrations of vitreous silica, α-quartz, α-cristobalite and Corning 7971 ultra-low expansion (ULE) glass have been measured from 1 to 20 kilobars using a diamond anvil type pressure cell. The mode Gruneisen parameters have been calculated. They showed unexpected negative values for the bond-stretching modes at 1100-1200 cm^{-1}. The values for bond-bending modes (750-800 cm^{-1}) and bond-rocking modes (450-480 cm^{-1}) are positive and negative respectively. The extra mode for ULE glass at 947 cm^{-1} showed an unexpected positive value. The relations between these values and their thermal expansion behaviours will be discussed.

*Work partially supported by the National Science Foundation and Advanced Research Projects Agency.

EE 7. An Accurate Interatomic Potential for Krypton. J. A. Barker, IBM Research, M. V. Bobetic, Univ. of Waterloo, and M. L. Klein, N.R.C.--An accurate interatomic potential for krypton is determined using high-energy molecular beam results, gas viscosities, second virial coefficients and zero-temperature crystal lattice spacing, cohesive energy and Debye theta. In calculating crystal properties, the Axilrod-Teller three-body interaction is included.[1] The potential is used to calculate other crystal properties (thermal expansion, elastic constants and specific heat up to 12°K) and other gas transport properties. Agreement with experiment is good. In particular the bulk modulus is only 3% higher than the X-ray experimental value.[2] For argon this discrepancy was 9%, and was tentatively ascribed[1] to the effect of the helium pressure fluid on lattice spacing. The present result adds some weight to this ascription, since the observed effect of helium on lattice spacing was also about three times smaller in krypton than in argon.

[1]M. V. Bobetic and J. A. Barker, Phys. Rev., in press.
[2]A. O. Urvas, D. L. Losee and R. O. Simmons, J. Phys. Chem. Solids 28, 2269 (1967).

EE 8. The Specific Heat of Sc_3In.* L. L. ISAACS and G. S. KNAPP, Argonne National Laboratory.--The specific heat of the weak ferromagnet Sc_3In has been measured in the temperature range of 0.6 to 4°K. The specimen of composition $Sc_{0.755}In_{0.245}$ has a Curie temperature of 6.7°K. The total measured specific heat has been decomposed into contributions due to the conduction electrons, the lattice and magnetic impurities. From the electronic specific heat coefficient (~20x10^{-3} J/mole°K^2), a density of states of 7 states/eV-atom at the Fermi level has been estimated. This is about twice the value for that of scandium.