Non rotating monochromatic single crystal X-ray (NORMOSIC) investigations of the sintal-phase intermetallic compound NaNi were undertaken for the first time. They show unusual and temperature dependent diffuse patterns. In addition to anisotropic thermal diffuse scattering close to Bragg peaks, extended off-Bragg regions of diffuse scattering are observed. (Fig. 1)

The interpretation is performed on the basis of lattice dynamical models which assume weak bonding of adjacent [110] zig-zag chains consisting of Na and Tl atoms respectively.

The study of the character of thermal vibrations is an important part in the dynamics of crystal lattice and is of principal value in the clarifying up the nature and real mechanisms of many physical phenomena in ferroelectrics. Certain conclusions about the presence of the thermal vibrations of ions were also defined on the perfect single crystal. The results obtained by this experiment on the whole confirmed the predictions of the anharmonicity of the vibrations of some ions and thereby to consider them to be ferroelectrically active. In the case of KTaO$_3$ the particularities of thermal vibrations of ions were also defined with very high accuracy with the help of the precise X-ray experiment which was carried out on the perfect single crystal. The results obtained by this experiment on the whole confirmed the qualitative conclusions which were made in the course of studying the polycrystalline samples of KTaO$_3$. The analysis of the further possibilities of studying the anharmonicity of the thermal vibrations on polycrystalline samples and single crystals of the above mentioned structural families was made.


The redetermination of the Avogadro constant currently in progress at the Physikalisch-Technische Bundesanstalt requires a relative uncertainty of less than 3 x 10^{-7} in the determination of the unit-cell volume in a silicon single crystal. From precision measurements of lattice spacings (Ando, Bailey, Hart, Acta Cryst. (1975) A31, 424) it is known that the shape of the unit-cell in highly pure silicon crystals is not exactly cubic. Thus the unit-cell volume, calculated from the knowledge of only one lattice plane spacing may exhibit a systematic error of up to 4 x 10^{-7}.

Using a whole set of 11 of equivalent lattice planes with $\sqrt{4 + k^2 + \ell^2} = const.$, the axial lengths a, b, c, axis angles $\alpha, \beta, \gamma$ and the volume v of a "real" unit-cell were calculated, assuming that the unit-cell is slightly deformed by internal or external forces.

By crystal-to-crystal comparison measurements, relative aberrations from the cubic shape in the order of $+ 2 \times 10^{-7}$ were found. The results are listed in the table. In order to study the differences in lattice plane spacings, this crystal wafers in a double crystal arrangement and consequent Laue reflections were used. Provided both wafers were of almost the same thickness, the rocking curves show a detailed fine structure which allows the differences in angular position to be detected to better than 10^{-6} rad.

In future work the mean unit-cell volume of a cube of silicon one kilogram in weight will be determined. Further investigation will be aimed at clarifying whether, as Ando, Bailey and Hart have surmised, the unit-cell volume in a highly pure silicon crystal remains almost constant.