05. PHYSICAL PROPERTIES AND STRUCTURE

05.2-7 OBSERVATION OF MAGNETOSTRICTIVE
ATOMIC SHIFTS IN NaF<sub>2</sub> FROM X-RAY DIFFRACTION DATA.
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Rutile-type NaF<sub>2</sub> was chosen to study the relationship between optical birefringence and structural change as a function of temperature in a simple antiferromagnet (T<sub>N</sub> = 87 K). It was previously inferred, on the basis of the Ewald-Born theory of structural birefringence, that a very small displacement of the fluorine ions would be sufficient to account for the observed magnetic contribution to the birefringence at first approximation, to relate nonlinear optical properties of a given crystal to the elastic behaviour of the crystal. The selection of NaF<sub>2</sub> for this study was based on the results of the work of the Heidelberg group. For NaF<sub>2</sub>, the second-order susceptibility tensor is greater than the number of independent components of nonlinear susceptibility tensor, so that a rough quantitative estimate of the maximum magnetic contribution can be made which reasonably agrees with the value experimentally determined.

05.2-8 THE ELASTIC CONSTANTS OF TARTARIC ACID.
By H. Küppers and M. Pies, Mineralogisches Institut,
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The elastic constants and their temperature coefficients of monoclinic tartaric acid were measured by an improved Schaefer-Bergmann method. A pulsed argon laser (50 Hz) was used, and the ultrasound was fed into the crystal only for a short time (100 ps) before the laser was triggered. This minimizes the warming up of the specimen by absorption of ultrasound.

The measured values c<sub>11</sub> = 75.4, c<sub>23</sub> = 16.0, c<sub>44</sub> = 35.2, c<sub>43</sub> = 8.4, c<sub>13</sub> = 16.0, c<sub>55</sub> = 11.1, c<sub>25</sub> = 8.0, c<sub>56</sub> = 12.7, c<sub>66</sub> = 8.9, c<sub>06</sub> = 20.3, c<sub>05</sub> = 0.5, c<sub>08</sub> = 3.8, c<sub>46</sub> = 0.2 · 10<sup>12</sup> dyn/cm<sup>2</sup> differ considerably from those determined by Mason (Piezoelectric crystals, 1950) by resonance techniques.

The elastic behaviour is characterized by an extreme anisotropy. The ratio of the maximum and minimum elastic stiffness is 5.9 : 1. This anisotropy can be correlated with the crystal structure (Okaya et al., Acta Cryst. 1966 B21, 237). The maximum stiffness is found parallel to the preferential direction of the hydrogen bonds. From spectroscopically determined molecular force constants a rough quantitative estimate of the maximum stiffness can be made which reasonably agrees with the value experimentally determined.

05.2-9 RELATION BETWEEN STRUCTURE AND PHYSICAL PROPERTIES OF NON-STOICHIOMETRIC TRANSITION METAL CARBIDES.
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The transition metals M of group III-VI can form carbides M<sub>C</sub> with NaCl lattice which are non-stoichiometric within the range 0.5 < x < 1. Short range order in the disordered high temperature modulated phases at x = 0.88 (V), 0.83 (V,Nb), 0.63 (Ti) and 0.5 (Ti<sub>2</sub>,Zr,ReC) can be described by a structure model considering repulsive interactions of carbon vacancies. Each carbon vacancy exhibits the same number of first, second and third nearest neighbours at compositions x = 1-x/2 (n = 0,1,...,12). The comparison of lattice energies for the resulting different structure models shows that short and long range ordering at x = 0.83 is favoured by a maximum of Coulomb energy, while covalent bond energy with a decrease of all NaCl bonds favours x = 0.5 and x = 1 compositions.

Some physical properties which are unusual for compounds with NaC<sub>1</sub> lattice can be described by the present structure model. The maxima of melting temperature, lattice constants, critical resolved shear stress and activation energies of diffusion at x = 0.8 can be correlated to the maximum Coulomb energy at x = 0.83.

a) Transition metal carbides with small lattice constants like VC<sub>1</sub> order at x = 0.83 and exhibit a large deviation from x = 1 stoichiometry because of the strong Coulomb interactions of carbon vacancies. The short range order parameters are close to those calculated for the structure model: a<sub>1</sub> = -0.7, a<sub>2</sub> = -0.2, a<sub>3</sub> = 0.2. The maximum carbon content of x = 0.89 can't only be achieved by >1% vacancies in the V sublattice similar as in Ti<sub>D</sub>. The carbon vacancies of VC<sub>0.88</sub> cannot be filled with hydrogen atoms.