If, assuming secondary extinction, a block size of 10^{-4} cm is obtained (small enough to assume no primary extinction) then a block size of 2×10^{-3} cm would be obtained assuming primary extinction, large enough to discount the existence of secondary extinction. Obviously, in this case the values of the mosaic block size deduced can in no way be used as a justification of the type of extinction assumed. The similarity of the mathematical corrections for the two kinds of extinction ensures that the agreement between the corrected and calculated structure factors would be the same for both. The mosaic block size obtained from the correction assuming primary extinction would be an order of magnitude larger than from that assuming secondary and would perhaps have a value more in keeping with the dislocation density values.

Identification of the type of extinction can only be done by testing the variation of extinction with path length, primary extinction being independent of the path length through the crystal. This can be examined either by using large crystals in which symmetry-related reflexions have different path lengths or by using many crystals of different sizes and the same mosaic character. It has been shown, Lawrence (1972, 1973), that both lithium fluoride and magnesium oxide suffer from primary extinction and Denne (1972), using α-glycine crystals of different sizes, showed that the amount of extinction in these crystals was independent of their shape and size, again suggesting primary extinction.

Doubts about the kind of extinction present must render the increasingly common use of the secondary extinction parameter refinement in a least-squares analysis physically meaningless. It must be again emphasized that little significance can be placed on extinction-corrected structure factors unless the correction is made experimentally.

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$Ni(NO_3)_2.6NH_3$, another example of KCN-type anomalous thermoelastic behavior.

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The temperature dependence of all elastic constants of cubic $Ni(NO_3)_2.6NH_3$, measured from the transition point at $-34{\cdot}2$ to 150°C by ultrasonic methods, exhibits KCN-type anomalous behaviour. Within a wide temperature range all elastic wave velocities increase with higher temperature. The shear resistance $c''=(c_{11}-c_{12})/2$ corresponds to the constant c_{44} in KCN. The change of c'' with absolute temperature obeys a logarithmic law like c_{44} in KCN, namely $c''=a\log T/T_0$ with $a=0{\cdot}05975\ .\ 10^{11}$ dyn cm^{-2} and $T_0=156{\cdot}22$°K. The anomalous elastic behaviour should be assigned mainly to the thermally activated motions of the NO_3 ions. The phase transition is directly related to the low c'' value.

Recently anomalous thermoelastic behaviour of cubic potassium cyanide was reported which is characterized by the following features (Haussühl, 1973):

(*a*) All elastic wave velocities increase with higher temperature over a wide temperature range.

(b) One elastic shear resistance (in KCN the elastic constant c_{44}) tends towards zero when approaching the transition point coming from higher temperatures according to $T_{44}=d(\log c_{44})/\mathrm{d}T=1/(T\log T/T_0)$, where T is temperature in °K and T_0 a specific constant.

(c) Bulk compressibility and also thermal expansion do not exhibit comparable anomalies in their temperature dependence.

With the older elastic and thermoelastic values of cubic $Ni(NO_3)_2.6NH_3$(NNA), which had been determined by ultrasonic pulse echo measurements in the vicinity of 0°C (Haussühl, 1963), a similar anomalous behaviour could only be suggested (Haussühl, 1973). Those measurements have now been expanded over a wider temperature range with higher precision in order to decide whether or not NNA behaves like KCN.

Measurements

The blue crystals of NNA, which had been grown from aqueous solutions by evaporation at a constant temperature of about 35°C to dimensions of several cm, undergo a phase transition at about $-34{\cdot}2$°C in agreement with earlier results of Jensen & Beevers (1938) and also of Long & Toettcher (1940) who found an anomaly in specific heat between -27 and -34°C with a maximum at $-29{\cdot}9$°C. Thomas, Staveley & Cullis (1952) observed a certain hysteresis which seems to depend on surface decomposition processes. The transition occurs spontaneously and is reversible. It is assigned to the order–disorder type of transition in which the orientation of the NO_3 ions is changing from an ordered arrangement to a statistically distributed multi-site arrangement similar to the motions of CN ions in KCN. The optical transparency of the crystals is lost during the transition by microcracks parallel to the cleavage faces {111}. In contrast to KCN the crystals did not regain their original transparency after retransition to higher temperatures. Up to about 170°C the crystals

Table 1. *Elastic constants* c_{ij}, *density* ϱ *of* $Ni(NO_3)_2.6NH_3$, $c' = (c_{11} + c_{12} + 2c_{44})/2$, $c'' = (c_{11} - c_{12})/2$

Units: c_{ij} in 10^{11} dyn cm^{-2}, ϱ in g cm^{-3}. In square brackets are the values $c''_{calc} = a \log T/T_0$ with $a = 0{\cdot}05975 \,.\, 10^{11}$ dyn cm^{-2} and $T_0 = 156{\cdot}22$°K.

T(°C)	c_{11}	c'	c_{44}	c''	c_{12}	ϱ
−34	0·9275	0·9719	0·0699	0·0255 [0·0254]	0·877	1·4911
−30	0·9279	0·9736	0·0721	0·0264 [0·0264]	0·875	1·4898
−20	0·9281	0·9769	0·0775	0·0287 [0·0288]	0·871	1·4868
0	0·9265	0·9816	0·0884	0·0333 [0·0334]	0·860	1·4809
20	0·9233	0·9844	0·0988	0·0377 [0·0376]	0·848	1·475
40	0·9187	0·9859	0·1090	0·0418 [0·0415]	0·835	1·4691
60	0·9127	0·9860	0·1188	0·0455 [0·0452]	0·822	1·4632
80	0·9060	0·9845	0·1275	0·0490 [0·0487]	0·808	1·4573
100	0·8985	0·9817	0·1352	0·0520 [0·0520]	0·795	1·4515
120	0·8905	0·9776	0·1414	0·0543 [0·0551]	0·782	1·4454
140	0·8822	0·9724	0·1458	0·0556 [0·0581]	0·771	1·4393
150	0·8779	0·9693	0·1472	0·0558 [0·0595]	0·766	1·4362

Table 2. *Thermoelastic constants* $T_{ij} = d(\log c_{ij})/dT$ *of* $Ni(NO_3)_2.6NH_3$

Unit: 10^{-3}/°C. In square brackets are the values $T''_{calc} = (T \log T/T_0)^{-1}$ with $T_0 = 156{\cdot}22$°K.

T(°C)	T_{11}	T'	T_{44}	T''	T_{12}
−30	0·06	0·38	7·3	8·8 [9·3]	−0·46
−20	−0·02	0·30	7·0	8·0 [8·2]	−0·55
0	−0·13	0·20	6·0	6·8 [6·6]	−0·66
20	−0·21	0·12	5·2	5·6 [5·4]	−0·73
40	−0·29	0·04	4·6	4·8 [4·6]	−0·79
60	−0·35	−0·04	3·9	4·0 [4·0]	−0·83
80	−0·40	−0·11	3·2	3·4 [3·5]	−0·85
100	−0·43	−0·17	2·6	2·5 [3·1]	−0·83
120	−0·46	−0·24	1·9	1·8 [2·8]	−0·76
140	−0·48	−0·30	1·2	0·7 [2·5]	−0·65
150	−0·49	−0·33	0·8	0·2 [2·4]	−0·59

possess surprisingly good stability if coated with a thin layer of paraffin oil. Above 170°C a slight decomposition starting at the surfaces begins. At about 200°C an apparently incongruent full decomposition with partial melting occurs. These processes are being more thoroughly investigated by Professor P.D.Garn.

The velocities of transverse and longitudinal elastic waves in the directions [100] and [110] were determined in the range −34·2 to 155°C by ultrasonic techniques, namely diffraction of light by ultrasonic waves at about 15 MHz (Schaefer-Bergmann method) and measuring the eigenfrequencies of thick plates. As optical light sources, argon ion lasers with the wavelengths 4880 and 4778 Å were employed. In this spectral range NNA is sufficiently transparent to give good diffraction photographs.

The necessary strong transverse waves could be excited in the crystals by reflexion of primary longitudinal waves at specially curved parts of the crystal surface. The results were controlled by pulse echo measurements which gave also a good accuracy for the temperature derivatives of the velocities of the transverse waves.

The values obtained for the three independent elastic constants, c_{11}, c_{12}, c_{44}, their temperature derivatives, and for the other directly observable elastic constants $c' = (c_{11} + c_{12} + 2c_{44})/2$ and $c'' = (c_{11} - c_{12})/2$ are presented in Table 1. The relative probable errors are within the following limits: c_{11}, c': 0·3%; c_{44}, c'': 0·6%. c_{12}: 1%. The values for the densities used in the evaluations are also included in Table 1. They were obtained using the known density at 20°C and the mean coefficient of linear thermal expansion $70 \,.\, 10^{-6}$/°C. Table 2 shows the logarithmic derivatives of the elastic constants as derived from the elastic data at various temperatures.

Discussion

The new measurements confirm that NNA exhibits KCN-type thermoelastic behaviour, showing also the above mentioned properties (*a*), (*b*) and (*c*). The temperature range in which these anomalies could be observed is smaller than in KCN owing to the higher transition temperature and the lower decomposition temperature of NNA. Concerning (*a*) one should note that the change in density lowers the constants T_{ij}, rather than the corresponding velocities, according to $T_{ij} = 2d(\log v_{ij})/dT + d(\log \varrho)/dT$, where v_{ij} are the velocities connected with the elastic constant c_{ij}. The velocities are therefore increasing in a wider temperature range than the corresponding elastic constants listed in Table 1.

The most affected shear resistance in NNA is $c'' = (c_{11} - c_{12})/2$. It belongs to the shear wave propagating in [110] with displacement vector parallel to [$\bar{1}$10]. As with KCN, this constant can be described by the simple formula $c'' = a \log T/T_0$ with $a = 0{\cdot}05975 \,.\, 10^{11}$ dyn cm^{-2} and $T_0 = 156{\cdot}22$°K; T is also in °K. This approximation represents the measured values in the range −34°C to about 100°C with a deviation of less than 1%. For T'' one obtains $T'' = 1/T \log T/T_0$, which shows stronger deviations from the experimental values only above 100°C.

These calculated values are also listed in Tables 1 and 2. At higher temperatures the bond-weakening contributions, which are mainly due to thermal expansion, govern the thermoelastic behaviour more and more.

Approaching the transition temperature from higher temperatures the constant c'' decreases to about $0{\cdot}0254 \,.\, 10^{11}$ dyn cm^{-2}. This low value can be compared with the corresponding constant for KCN, c_{44}, which reaches $0{\cdot}01926 \,.\, 10^{11}$ dyn cm^{-2} in the vicinity of the transition temperature.

To a first approximation one may relate these values to the thermal induction of critical shear strains leading to a breakdown of the high temperature phase. Assuming nearly equal critical shear strains for both NNA and KCN, $c''(\mathrm{NNA})/T_t(\mathrm{NNA})$ and $c_{44}(\mathrm{KCN})/T_t(\mathrm{KCN})$, where T_t is the absolute transition temperature, will represent comparable critical values for the stability of the high-temperature phase. One obtains $c''(\mathrm{NNA})/T_t(\mathrm{NNA}) = 0{\cdot}0254/238{\cdot}9 \approx 1{\cdot}06 \,.\, 10^{-4}$dyn cm^{-2}/°C and $c_{44}(\mathrm{KCN})/T_t(\mathrm{KCN}) = 0{\cdot}01926/167{\cdot}6 \approx 1{\cdot}15 \,.\, 10^{-4}$ dyn cm^{-2}/°C.

The small difference in these values and the other common properties of KCN and NNA lead to the conclusion that the same kind of thermally activated interaction is responsible for the stability of the high-temperature phases and the anomalous thermoelastic behaviour. In KCN the essential part of this anomaly should be assigned to the librational motions and orientational jumping processes of the CN dipoles and the interaction between the adjacent dipoles. As was suggested by Kraceck, Hendricks & Posnjak (1931), the NO_3 ions in NNA must rotate at room temperature in order to comply with the X-ray data. At present one cannot decide whether or not the librational and orientational motions of the NO_3 ions alone are responsible for the effects observed in NNA. A contribution from similar motions of the NH_3 groups should be also discussed. Until now a satisfying model giving a quantitative interpretation of the elastic behaviour could not be established, but there can be no doubt that in KCN and NNA a special type of interaction is revealed in an exceptionally pure form. One can assume that in many other materials such interactions occur, sometimes strongly screened by the usual contributions which weaken the elastic bonds with increasing temperatures.

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Multiple scattering and dynamical effects in diffuse electron scattering: errata.

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Corrections are given to *Acta Cryst.* (1973). A**29**, 663–672.

Printing errors have been found in the article by Høier (1973). The corrections are given below.

The integrals in equation (9), $\int \exp(-\mu^j z) P_1(z) \mathrm{d}z$ and $\int \exp(-\mu^j z) P_n(z) \mathrm{d}z$, should read respectively $\int \exp(\mu^j z) P_1(z) \mathrm{d}z$ and $\int \exp(\mu^j z) P_n(z) \mathrm{d}z$.

The sentence on page 666, second column, first line '– – – by a power expansion in $\Delta\mu^j t$:' should be replaced by '– – – by a power expansion in $\Delta\mu^j t$; including the prefactor $\exp(-\mu^j t)$ we get:'

Equation (11) $A_n = W_n(z)$ should read $A_n = W_n(t)$.

The function $g(z) = \exp(-\mu z) P_n(z)$ on page 667, first column, line 5 should read $g(z) = \exp(\mu z) P_n(z)$. A corresponding change in $g(z)$ should be introduced in the caption of Fig. 2.

Reference

HØIER, R. (1973). *Acta Cryst.* A**29**, 663–672.