

$$\begin{aligned}
 &= \frac{e^{iR\phi}}{F(e^{i\phi})} \sum_{r=0}^{R-1} \left(\sum_{m=0}^{R-1-r} a_m e^{-i(m+r)\phi} \right) \sum_{v=1}^{\sigma} T_r^{(v)}. \\
 \therefore \quad \sum_{v=1}^{\sigma} D'_v(\phi) &= \frac{\sum_{n=0}^{R-1} \left(\sum_{m=0}^n a_m T_{n-m} \right) e^{-in\phi}}{\sum_{n=0}^R a_n e^{-in\phi}} \quad (88)
 \end{aligned}$$

which is equivalent to equations (35) and (45).

References

ALLEGRA, G. (1961). *Acta Cryst.* **14**, 535.
 ALLEGRA, G. (1964). *Acta Cryst.* **17**, 579.
 GEVERS, R. (1952). *Acta Cryst.* **5**, 518.
 GEVERS, R. (1954a). *Acta Cryst.* **7**, 337.
 GEVERS, R. (1954b). *Acta Cryst.* **7**, 492.
 HENDRICKS, S. & TELLER, E. (1942). *J. Chem. Phys.* **10**, 147.
 JAGODZINSKI, H. (1949a). *Acta Cryst.* **2**, 201.
 JAGODZINSKI, H. (1949b). *Acta Cryst.* **2**, 208.
 JAGODZINSKI, H. (1949c). *Acta Cryst.* **2**, 298.
 JAGODZINSKI, H. (1954). *Acta Cryst.* **7**, 17.
 KAKINOKI, J. & KOMURA, Y. (1952). *J. Phys. Soc. Japan*, **7**, 30.
 KAKINOKI, J. & KOMURA, Y. (1954a). *J. Phys. Soc. Japan*, **9**, 169.
 KAKINOKI, J. & KOMURA, Y. (1954b). *J. Phys. Soc. Japan*, **9**, 177.
 KAKINOKI, J. & KOMURA, Y. (1962). *Acta Cryst.* **15**, 292.
 KOMURA, Y. (1962). *Acta Cryst.* **15**, 770.
 MÉRING, J. (1949). *Acta Cryst.* **2**, 371.
 PATERSON, M. S. (1952). *J. Appl. Phys.* **23**, 805.
 WARREN, B. E. & WAREKOIS, E. P. (1955). *Acta Metallurg.* **3**, 473.
 WARREN, B. E. (1959). *Prog. Met. Phys.* **8**, 147.
 WILSON, A. J. C. (1942). *Proc. Roy. Soc., A*, **180**, 277.
 WILSON, A. J. C. (1943). *Proc. Roy. Soc., A*, **181**, 360.
 ZACHARIASEN, W. H. (1947). *Phys. Rev.* **71**, 715.

Short Communications

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Antiferromagnetism in nickel orthosilicate*. By R. NEWNHAM, R. SANTORO, J. FANG† and S. NOMURA‡, *Electrical Engineering Dept., Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A.*

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Nickel orthosilicate, Ni_2SiO_4 , is isomorphous with the mineral olivine. Polycrystalline specimens were prepared from sodium orthosilicate and nickel nitrate. After the components were dissolved separately in distilled water, the orthosilicate solution was slowly added to the nitrate solution, yielding a hydrated nickel silicate precipitate. The precipitate was filtered and washed, and then fired at 1400°C for 24 hours to give Ni_2SiO_4 . Least-squares refinement of high-angle X-ray diffractometer data gave the lattice parameters $a = 10.121 \pm 0.005$, $b = 5.915 \pm 0.002$, $c = 4.727 \pm 0.002 \text{ \AA}$. The space group is $Pnma$ with four formula-units per unit cell.

A vibrating-sample magnetometer was used to measure the magnetic susceptibility of Ni_2SiO_4 . As shown in Fig. 1, the susceptibility follows a Curie-Weiss law above 60°K , with $\Theta = 7^\circ\text{K}$ and $p_{\text{eff}} = 3.15 \mu_B$. Kondo & Miyahara (1963) report slightly different values of -14°K and $3.04 \mu_B$. The susceptibility goes through a maximum near 34°K , indicative of a paramagnetic-antiferromagnetic transition.

Neutron diffraction patterns of polycrystalline Ni_2SiO_4 taken above and below the Néel temperature are shown in Fig. 2. The nuclear intensities (Table 1) agree well with values calculated from the olivine coordinates (Hanke & Zemann, 1963), confirming the crystal structure. The magnetic peaks in the low-temperature pattern cannot be in-

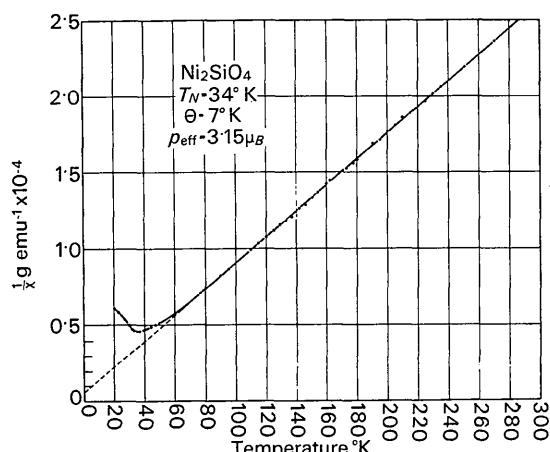


Fig. 1. The reciprocal susceptibility of Ni_2SiO_4 plotted as a function of temperature.

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Table 1. Comparison of observed and calculated nuclear intensities indexed on the chemical unit cell.

<i>hkl</i>	<i>d_{calc}</i>	<i>I_{calc}</i>	<i>I_{obs}</i>	<i>d_{obs}</i>
200	5.06	3	2	5.08
101	4.28	4	6	4.29
210	3.85	5	4	3.86
011	3.69	3	3	3.71
111	3.47	25	30	3.48
201	3.45	2		
211	2.98	2		
020	2.96	2	4	2.98
301	2.75	35	30	2.76
220	2.55	4	6	2.56
400	2.53	2		
311	2.49	22	26	2.49
121	2.43	39	36	2.44

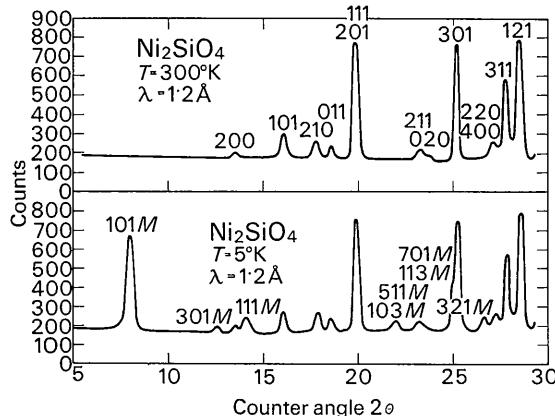


Fig. 2. Neutron diffraction powder patterns of Ni_2SiO_4 taken above and below the antiferromagnetic transition. Indices for the nuclear intensities are given in the room-temperature pattern. The magnetic reflections (*M*) in the low-temperature pattern are indexed on an orthorhombic magnetic cell with dimensions $20.2 \times 5.9 \times 9.5 \text{ \AA}$.

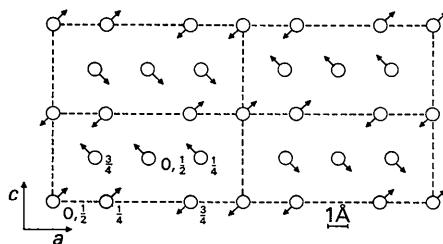


Fig. 3. Possible spin arrangement in antiferromagnetic Ni_2SiO_4 projected on (010). Heights of the Ni ions are expressed in cell fractions; silicon and oxygen positions are not shown. The magnetic superlattice and four chemical sub-cells are outlined.

dexed on the chemical unit cell and require a $2a \times b \times 2c$ superlattice cell containing 32 nickel atoms. This many spin directions cannot be established with certainty from the powder diagram, but the antiferromagnetic alignment in Fig. 3 gives reasonable agreement with experiment (Table 2). The computational methods outlined by Shirane (1959) proved useful in calculating the magnetic intensities.

Table 2. Comparison of observed and calculated magnetic intensities indexed on the magnetic superlattice

<i>hkl</i>	<i>d_{calc}</i>	<i>I_{calc}</i>	<i>I_{obs}</i>	<i>d_{obs}</i>
101	8.57	33	36	8.60
301	5.51	1	3	5.49
111	4.87	6	7	4.88
311	4.03	1	<2	—
501	3.72	1	<2	—
511	3.15	2	3	3.14
103	3.12	2		
303	2.86	0	<2	—
121	2.80	0	<2	—
701	2.77	2		
113	2.76	1	2	2.77
321	2.60	6	5	2.60
711	2.51	0	<2	—

The model was derived from the magnetic structure of cobalt orthosilicate (Nomura, Santoro, Fang & Newnham, 1964), in which spins at height $z=0$ in the chemical cell are antiparallel to those at $z=\frac{1}{2}$. The cobalt moments are collinear with **b**. When indexed on the quadrupled cell, the magnetic reflections of Ni_2SiO_4 are absent unless *h* and *l* are odd, suggesting that spins related by translational vectors along **a** and **c** are antiparallel. Intensity calculations were carried out for a number of four-spin models similar to the Co_2SiO_4 arrangement and consistent with the *B*-face centering condition. The best results were achieved with the spins in (010), as indicated in Fig. 3. Within this plane only relative spin directions can be determined from the powder pattern; rotation of the entire spin system about **b** yields identical intensities.

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References

HANKE, K. & ZEMANN, J. (1963). *Naturwissenschaften*, **50**, 91.
 KONDO, H. & MIYAHARA, S. (1963). *J. Phys. Soc. Japan*, **18**, 305.
 NOMURA, S., SANTORO, R., FANG, J. & NEWNHAM, R. (1964). *Phys. Chem. Solids*, **25**, 901.
 SHIRANE, G. (1959). *Acta Cryst.* **12**, 282.