



Figure 9 The influence of the atactic content and the spherulite diameter in PP on the band initiation stress σ_{BI} at various temperatures, T . With increasing temperature (-196 to -50°C) the discrete shear band deformation develops into a more homogeneous deformation along a broad shear zone.

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The crystal structure of the silicon cerium oxynitride, $\text{Ce}_4\text{Si}_2\text{O}_7\text{N}_2$

In an investigation on the densification of Si_3N_4 with CeO_2 , Mah *et al.* [1] have reported the existence of a new quaternary compound in the system Ce–Si–O–N having a chemical formula of $\text{Ce}_4\text{Si}_2\text{O}_7\text{N}_2$, the powder diffraction pattern of which has been indexed on the basis of a monoclinic unit-cell with dimensions: $a = 10.360 \text{ \AA}$, $b = 10.865 \text{ \AA}$, $c = 3.974 \text{ \AA}$ and $\beta = 90.33^\circ$. However, the crystal structure proposed by these

workers cannot be correlated with any known compound. While the existence of a compound with the proposed chemical composition is beyond doubt, there seems to be a discrepancy in the indexing of the powder diffraction pattern and assignment of correct unit-cell parameters for the compound.

Earlier studies on the crystal structure determination of a number of silicon–lanthanide-oxynitrides of the general formula $\text{Ln}_4\text{Si}_2\text{O}_7\text{N}_2$ ($\text{Ln} = \text{La, Nd, Sm, Gd, Dy, Ho, Er}$ and Yb) have been carried out independently by Wills *et al.* [2]

TABLE I X-ray diffraction data for $Ce_4Si_2O_7N_2^*$

I/I_0	$d_{obs.}$	$d_{calc.}$	$h k l$
25	7.506	7.500	0 1 1
4	5.434	5.432	0 2 0
2	5.187	5.181	0 0 2
8	4.821	4.811	0 2 1
30	4.677	4.677	0 1 2
8	3.750	3.749	0 2 2
1	3.705	3.701	2 0 $\bar{2}$
1	3.512	3.517	2 1 0
4	3.419	3.419	0 3 1
30	3.291	3.292	0 1 $\bar{3}$
100	3.209	3.207	2 2 $\bar{1}$
10	3.068	3.068	2 2 0
8	3.061	3.060	2 2 $\bar{2}$
14	3.037	3.036	2 1 1
14	3.022	3.020	2 1 $\bar{3}$
35	2.968	2.968	0 3 2
40	2.915	2.915	0 2 3
5	2.718	2.716	0 4 0
8	2.627	2.627	0 4 1
8	2.613	2.615	2 0 2
8	2.600	2.598	2 0 $\bar{4}$
4	2.589	2.590	0 0 4
		2.588	2 3 $\bar{2}$
2	2.543	2.542	2 1 2
1	2.529	2.527	2 1 $\bar{4}$
1	2.519	2.520	0 1 4
1	2.409	2.407	1 4 $\bar{2}$
		2.406	3 1 $\bar{3}$
3	2.382	2.382	2 3 1
2	2.374	2.373	2 3 $\bar{3}$
6	2.242	2.242	2 4 $\bar{1}$
		2.127	3 3 $\bar{1}$
2	2.127	2.126	0 5 1
6	2.120	2.120	2 3 2
6	2.112	2.111	2 3 $\bar{4}$
4	2.061	2.060	2 4 $\bar{1}$
3	2.055	2.055	2 4 $\bar{3}$
10	2.035	2.035	0 1 5
1	2.019	2.020	2 2 3
16	1.987	1.986	4 0 $\bar{2}$
1	1.936	1.936	0 2 5

*Monoclinic: $a = 7.946 \text{ \AA}$, $b = 10.865 \text{ \AA}$, $c = 11.075 \text{ \AA}$ and $\beta = 110.65^\circ$.

and Marchand *et al.* [3] who reported that the X-ray diffraction patterns for these compounds can be indexed on the basis of a monoclinic unit-cell similar to that of the compound cuspidine, $Ca_4Si_2O_7F_2$ (space group $P2_1/c$). A yttrium analogue, $Y_4Si_2O_7N_2$ has also been reported by Wills *et al.* [4] with a similar structure to that of

the cuspidine. Thus it can be expected that the Ce^{3+} analogue of the silicon-lanthanide-oxynitrides would behave similarly and exhibit the same type of crystal structure. The purpose of the present communication is to show that a very satisfactory refinement can be obtained from the X-ray powder data of $Ce_4Si_2O_7N_2$ based on a monoclinic unit-cell which bears a close resemblance to those of the lanthanide and yttrium analogues with cuspidine structure.

The measured and calculated d -values for $Ce_4Si_2O_7N_2$ with the corresponding relative intensities are given in Table I. The X-ray data reported here are based on the basis of a monoclinic unit-cell with dimensions: $a = 7.946 \text{ \AA}$, $b = 10.865 \text{ \AA}$, $c = 11.075 \text{ \AA}$ and $\beta = 110.65^\circ$.

It is noteworthy that the indexing obtained with the above cell parameters are in good agreement with those reported for cuspidine and the relative intensities are comparable to one another. As can be expected the various known silicon-lanthanide-oxynitrides show a progressive increase in the unit-cell parameters with increasing ionic radii of the lanthanide cation. The cell parameters proposed for $Ce_4Si_2O_7N_2$ appear to be consistent with this behaviour.

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