Pure Appl. Chem., Vol. 71, No. 9, pp. 1765–1769, 1999.
Printed in Great Britain.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

INORGANIC CHEMISTRY DIVISION
COMMISSION ON HIGH TEMPERATURE MATERIALS AND SOLID STATE CHEMISTRY

TERMINOLOGY FOR COMPOUNDS IN THE Si-Al-O-N SYSTEM

(IUPAC Recommendations 1999)

Prepared for publication by
R. METSELAAR[1] AND D. S. YAN[2]

[1]*Laboratory of Solid State Chemistry and Materials Science, Technische Universiteit Eindhoven, Postbus 513, NL-5600 MB Eindhoven, Netherlands*
[2]*Shanghai Institute of Ceramics, Academia Sinica, 1295 Ding-Xi Road, Shanghai 200050, China*

Terminology for compounds in the Si-Al-O-N system (IUPAC Recommendations 1999)

Abstract: This document proposes a nomenclature for aluminium silicon oxide nitrides [In ceramic literature these compounds are generally called oxynitrides. According to IUPAC rules (cf. G. J. Leigh, ed. *Nomenclature of Inorganic Chemistry*. Blackwell Scientific Publishers, Oxford, UK (1990)) this is not allowed; the systematic name should be oxide nitride or oxonitride].

INTRODUCTION

Silicon and aluminium containing nitrides and oxide nitrides are widely studied by the chemical and ceramic community because of the interesting applications, in particular related to their (thermo-)mechanical properties. In the many publications on these materials several abbreviations are used to designate the materials. These relate in part to the processing technology in part to the composition. In the materials community at large and in the ceramic community in particular it is tried to reach agreement upon the use of such acronyms. In the interest of maintaining uniformity in the chemical terms a proposal is made here.

Abbreviations

In literature one finds many abbreviations for compounds in the Si-Al-O-N system. Examples are B, D, E, H, J, JEM, K, M, M′, O, Q, U, X and others. Since nowadays the chemical composition and crystal structure are known for most of these compounds, the use of such nonself-explaining abbreviations is discouraged. A general nomenclature on solids is available [1]. If abbreviations are used, they should always be defined once in any paper, and they should generally be avoided in titles and abstracts.

Prime-sign

In literature one finds the use of a prime sign in combination with an abbreviation, e.g. α′-sialon, O′-sialon, etc. In literature this is often used to indicate a phase with (a) the same structure as the parent phase, but (b) a different composition and (c) forming no solid solution with the parent phase. As mentioned above, the use of abbreviations should be avoided where possible and the same holds for the combination with a prime. The use of the prime can be convenient in phase diagrams. An example is the use of the symbol α′ to indicate the phase field of α-sialon in a phase diagram with the parent α-Si_3N_4 phase. However, the use in cases where a continuous solid solution is formed with the parent phase is only confusing.

Concentration units

Concentrations in compounds with the general formula $Si_aAl_bO_cN_d$, so called sialons, are sometimes given in (charge) equivalent percents. For instance the equivalent percentage of Si in this formula is $100\times 4a/(4a+3b)$, the equivalent percentage of N is $100\times 3d/(2c+3d)$.

A related notation is β_y, where y denotes the eq% of Al. For instance $Si_2Al_4O_4N_4$, corresponding to $x=4$ in the composition $Si_{6-x}Al_xO_xN_{8-x}$, contains 60 eq.% of Al and is then indicated by β_{60}. This notation is not self-explaining and is not encouraged.

TERMS FOR COMPOUNDS IN THE SI-AL-O-N SYSTEM

alon

A generic name for compounds or solid solutions in the system Al-O-N (The use of capitals as in AlON is discouraged since they suggest a chemical composition).

γ-alon

A solid solution in the Al_2O_3-AlN system centred around the composition $AlN.3Al_2O_3$, with spinel type structure.

alon polymorphs

A series of polymorphic compounds [2] in the alon system of composition M_mX_{m+1} with M = Al and X = N, O. Compounds have been reported with $m = 6$, 7, 8, 9, 10. They are layered structures with Ramsdell symbols 12H, 21R, 16H, 27R, 20H, respectively.

sialon

A generic name for compounds or solid solutions in the system M-Si-Al-O-N, where M is a metal. (The use of capitals as in SiAlON is discouraged since they suggest a chemical composition).

α-sialon

A solid solution of composition $M_{m/v}Si_{12-(m+n)}Al_{m+n}O_nN_{16-n}$ with the structure of α-Si_3N_4; where M is an element with valency v, such as Li, Ca, Y and many of the rare earth ions, m and n vary between various limits depending on the element M and the temperature. Sometimes symbols α and α′ are used to indicate α-Si_3N_4 and α-sialon, respectively. The main reason for this is that α-sialon has the same structure as α-Si_3N_4, but does not form a continuous solid solution with the latter. Although this can be of use in a phase diagram, the use in texts of α′-sialon instead of α-sialon is not recommended unless one wants to emphasise this difference.

β-sialon

A solid solution of composition $Si_{6-x}Al_xO_xN_{8-x}$ with the structure of β-Si_3N_4, where x varies between 0 and about 4.2 (depending on temperature). The use of β′-sialon instead of β-sialon is discouraged.

sialon polymorphs

A series of polymorphic compounds [2] in the sialon system of composition M_mX_{m+1} with M = Al, Si and X = N, O. Compounds have been reported with $m = 4$, 5, 6, 7, 9, 11. They are layered structures with Ramsdell symbols 8H, 15R, 12H, 21R, 27R, $2H^{\delta}$. Approximate compositions of the main polymorphs are $SiAl_4O_2N_4$ (15R), $SiAl_5O_2N_5$ (12H), $SiAl_6O_2N_6$ (21R), $SiAl_8O_2N_8$ (27R). Note: elements Be, Mg, Sc and possibly other cations can be incorporated in these structures provided that charge balance is preserved and that the overall M:X ratio is retained.

α-Si_3N_4

A crystalline type of silicon nitride with spacegroup P31*c*.

β-Si_3N_4

A crystalline type of silicon nitride with spacegroup $P6_3/m$ or $P6_3$.

SN

An abbreviation used for silicon nitride, Si_3N_4. This term should never be used as an abbreviation for the compound as such. It is, however, regularly used as an initialism in combination with a processing prefix. An example is RBSN, which stands for reaction bonded silicon nitride. These terms are not considered in this manuscript, but they are under consideration by committees on standardisation.

SNO

Silicon oxide nitride, Si_2ON_2. The use of the abbreviation SNO is strongly discouraged. The compound is also indicated by the abbreviation O-phase or O-sialon (see below).

Single letter abbreviations

The following alphabetical list gives examples found in literature (not exhaustive). As mentioned above, the use of these nondescriptive terms should be avoided where possible.

B-phase: Y_2SiAlO_5N

D-phase: $YSi_2AlO_4N_2$

E-phase: YSi_3O_6N. A compound with the β-$Y_2Si_2O_7$ type structure.

H-phase: A solid solution derived from $Ln_5Si_3O_{12}N_1$ with apatite type structure, where Ln = Y or a lanthanide ion. The compound $Ln_5Si_3O_{12}N_1$ is also called N-apatite in some papers, however, this is not recommended.

J-phase: A solid solution of composition $Ln_4Si_{2-x}Al_xO_{7+x}N_{2-x}$, with x between 0 and 2, with cuspidine type structure where Ln = Y or a lanthanide ion.

J′-phase: $Si_3Al_3O_{3+1.5x}N_{5-x}$ a term used in older literature and not related to the J-phase.

JEM-phase: A solid solution of composition $LnSi_{6-x}Al_{1+x}N_{10-x}O_x$, with $x \approx 1$, isomorphous with $LaSi_3N_5$, and Ln = Y or a lanthanide ion.

K-phase: A solid solution derived from $Ln_3Si_3O_6N_3$ with wollastonite type structure where Ln = Y or a lanthanide ion.

M-phase: In earlier literature used for the compound $Ln_2Si_3O_3N_4$, with melilite type structure (sometimes called N-melilite), where Ln = Y or a lanthanide ion. Now often used for solid solutions of composition $Ln_2Si_{3-x}Al_xO_{3+x}N_{4-x}$, with x between 0 and 1. Some authors use M′-phase to indicate this solid solution. The use of the prime sign is discouraged.

O-phase: A solid solution of composition $Si_{2-x}Al_xO_{1+x}N_{2-x}$, where x varies between 0 and about 0.3. Some authors use O-phase for the compound with $x = 0$ and O′ for the solid solution. The use of the prime sign is discouraged. In older literature this phase has also been called X-phase. Since it is a very prominent phase in many sialon compositions many authors find it convenient to retain the name O-phase.

Q-phase: The 12H sialon polymorph with $m = 6$ (see above)

U-phase: A solid solution $Ln_3Si_{3-x}Al_{3+x}O_{12+x}N_{2-x}$, with x between 0 and 1, of $La_3Ga_5SiO_{14}$ structure type.

W-phase: $Ln_4Si_9Al_5O_{30}N$, where Ln = Y or a lanthanide ion.

Y-phase: The 15R sialon polymorph with $m = 5$ (see above)

X-phase: A compound in the Si-Al-O-N system with a narrow solubility region. There are several approximate compositions in literature, centred around a composition $Si_{10}Al_{15}O_{32}N_7$. Since the structure type is unknown and given the uncertainties in composition the use of the term X-phase is convenient for the time being.

Z-phase: $Y_3Si_2ON_5$

ϵ-phase: $SiAl_7O_2N_7$

η-phase: $SiAl_3O_2N_3$

θ-phase: $Si_3Al_{12}O_9N_{10}$

ζ-phase: $Si_3Al_7O_3N_9$

ACKNOWLEDGEMENTS

Suggestions and comments made by the following during compilation of this document are gratefully acknowledged: I.W.M. Brown, I-Wei Chen, Y-B. Cheng, A. Hendry, H.T. Hintzen, M.J. Hoffmann, K. Jack, S-J.L. Kang, H. Mandal, R. Marchand, M. Mitomo, D. Niesz, M. Sopicka-Lizer, D.P. Thompson, T-Y. Tien and J. Zheng.

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