

“Martensite Type” FeC_x ($x < 0.06$) ($L'2_0$) Structure: AB_tI4_139_a_b-002

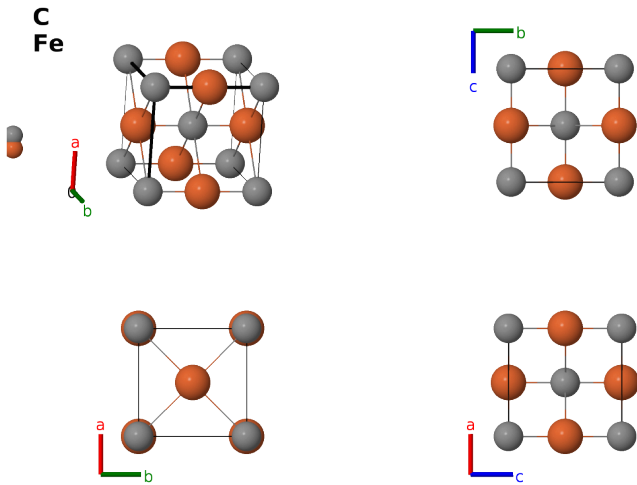
This structure previously used the label(s) **AB_tI4_139_b_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/ZN4Y>

https://aflow.org/prototype-encyclopedia/AB_tI4_139_a_b-002



Prototype	C_xFe
AFLOW prototype label	AB.tI4_139_a_b-002
<i>Strukturbericht</i> designation	$L'2_0$
Pearson symbol	tI4
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	<code>aflow --proto=AB_tI4_139_a_b-002 --params=a, c/a</code>

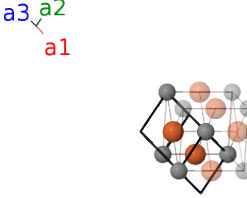
Other compounds with this structure

FeN_x

- This should *not* be considered a true model of martensite, a very complex material whose structure is sensitive to composition (Blackwell, 1996; Sherby, 2008). However, (Ewald, 1931) assign this the label $L'2_0$, saying that this structure is “ α -Fe with 6 atomic percent C.” Although (Ewald, 1931) present a long discussion of martensite (pp. 489, 576-583), they do not give this exact crystal structure, which we take from (Brandes, 1992) and (Pearson, 1967).

- (Villars, 1995) and (Westbrook, 1995) ignore this structure and give the $L'2$ label to the ThH_2 structure. We previously followed this notation, but in the interest of historical accuracy will relabel that structure with the name given to it by (Brandes, 1992) and (Pearson, 1967), $L'2_b$.
- We should note that these last two references list the current structure simply as $L'2$.
- $L'2_0 \text{ FeC}_x$ and $\beta\text{-LiFeO}_2$ have the same AFLOW prototype label, AB_tI4_139_a_b. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}
 \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) C I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2b) Fe I

References

- [1] E. A. Brandes and G. B. Brook, eds., *Smithells Metals Reference Book* (Butterworth Heinemann, 1992), chap. 6, pp. 6–63, 7e edn.
- [2] R. Blackwell, *Internal Friction Effects in Tempered Martensite*, *Nature* **211**, 733–734 (1966), doi:10.1038/211733a0.
- [3] O. D. Sherby, J. Wadsworth, D. R. Lesuer, and C. K. Syn, *Revisiting the Structure of Martensite in Iron-Carbon Steels*, *Mater. Trans.* **49**, 2016–2027 (2008).
- [4] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.
- [5] J. H. Westbrook and R. L. Fleischer, eds., *Intermetallic Compounds – Principles and Practice* (John Wiley & Sons, Ltd., Chichester, England, 1995). Two Volumes.
- [6] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2, International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).

Found in

- [1] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).

First cited in

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