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

This structure originally had the label `AB_tI4_139_b_a`. Calls to that address will be redirected here.

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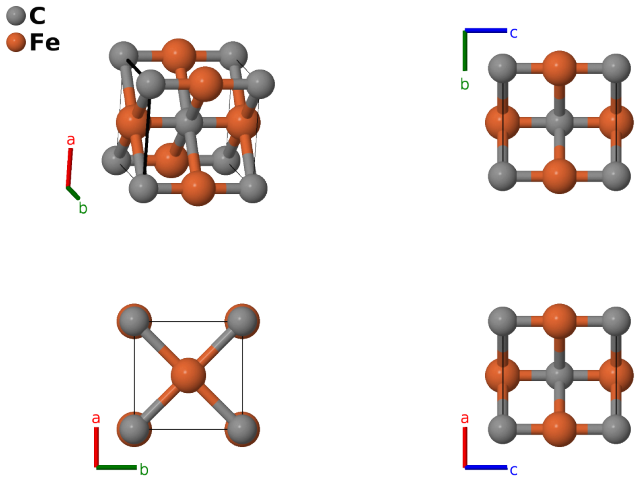
https://aflow.org/p/ZN4Y

https://aflow.org/p/AB_tI4_139_a_b-002



Prototype	C_xFe
AFLOW prototype label	AB_tI4_139_a_b-002
***Strukturbericht* designation**	$L'2_0$
ICSD	none
Pearson symbol	tI4
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=AB_tI4_139_a_b-002 --params=`$a, c/a$

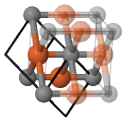
Other compounds with this structure
FeN_x

- 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 $L'2$.
- $L'2_0$ FeC_x and β-$LiFeO_2$ 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

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



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).