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# Revisiting the five-decade-old structure of the $Fe_2WO_6$ powder with incommensurate modulations

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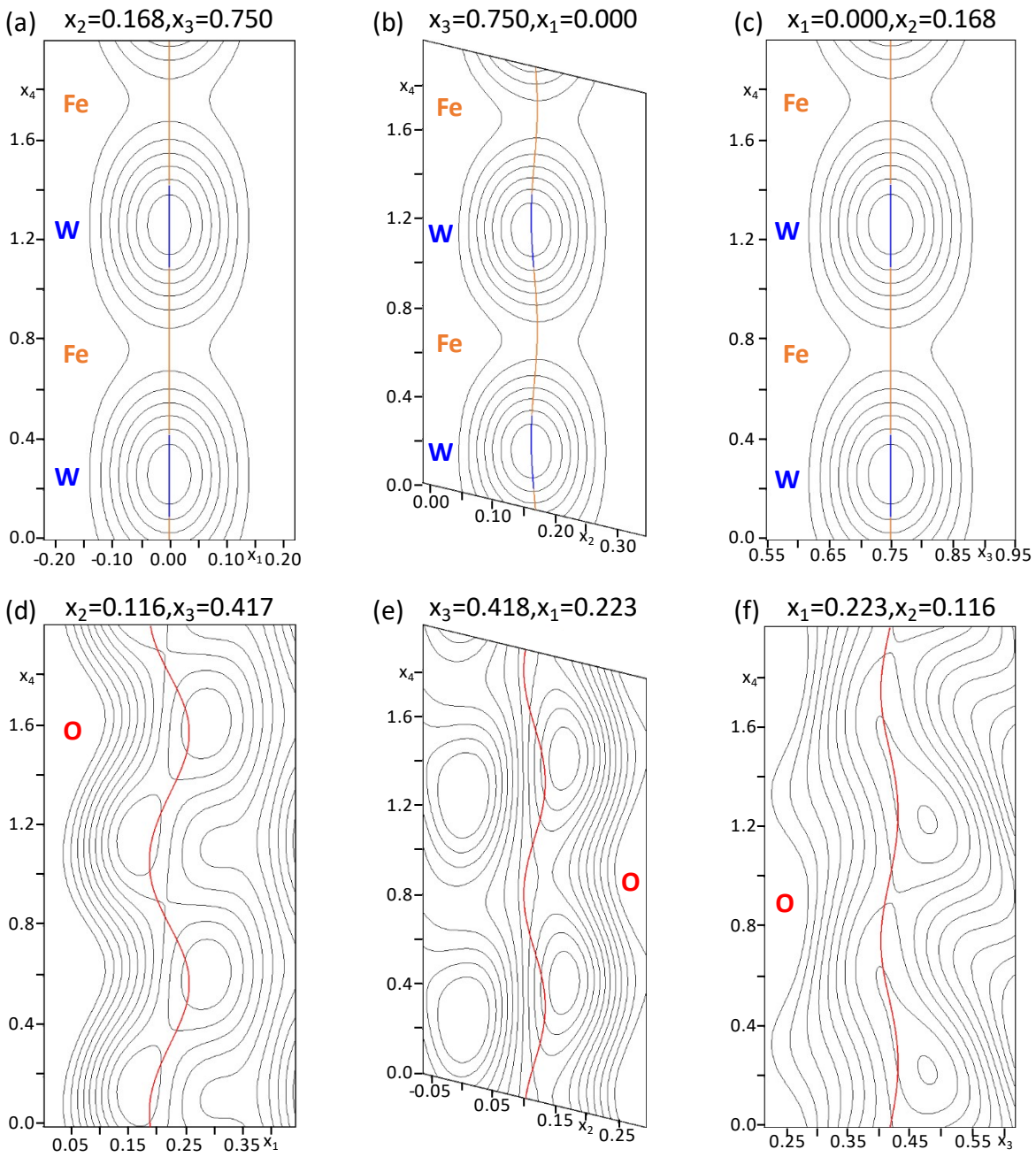


Figure S1. De Wolff $x_1$–$x_4$, $x_2$–$x_4$ and $x_3$–$x_4$ sections showing the occupational and positional modulations of Fe, W and O in $Fe_2WO_6$ ceramic sample as a function of the internal $x_4$ axis calculated in the vicinity of the atomic position ($x_1 = x$, $x_2 = y$, $x_3 = z$). The central colored lines correspond to the calculated atomic positions (orange: Fe; blue: W, red: O).

Table S1. Selected interatomic distances (Å) and bond valence sums (BVS) in the modulated structure of $Fe_2WO_6$ ceramic sample.

| | Average | Minimum | Maximum |
|---|---|---|---|
| Fe1-O1$^{i}$ | 2.01(2) | 1.87(3) | 2.08(3) |
| Fe1-O1$^{ii}$ | 1.99(2) | 1.84(3) | 2.08(3) |
| Fe1-O1$^{iii}$ | 2.01(2) | 1.87(3) | 2.08(3) |
| Fe1-O1$^{iv}$ | 1.99(2) | 1.84(3) | 2.08(3) |
| Fe1-O1$^{v}$ | 2.13(3) | 1.97(3) | 2.22(3) |
| Fe1-O1$^{vi}$ | 2.13(3) | 1.97(3) | 2.22(3) |
| W1-O1$^{i}$ | 1.88(2) | 1.85(3) | 1.95(3) |
| W1-O1$^{ii}$ | 1.83(2) | 1.80(3) | 1.91(3) |
| W1-O1$^{iii}$ | 1.88(2) | 1.85(3) | 1.95(3) |
| W1-O1$^{iv}$ | 1.83(2) | 1.80(3) | 1.91(3) |
| W1-O1$^{v}$ | 1.94(2) | 1.91(3) | 2.00(3) |
| W1-O1$^{vi}$ | 1.94(2) | 1.91(3) | 2.00(3) |
| | | | |
| BVS Fe1 | 2.902(7) | 2.33(2) | 3.97(2) |
| BVS W1 | 6.57(3) | 5.78(2) | 7.03(2) |
| BVS O1 | 2.063(8) | 1.67(2) | 2.44(2) |

Symmetry codes: (i) $x_1, x_2, x_3, x_4$; (ii) $-x_1+1/2, -x_2+1/2, x_3+1/2, -x_4$; (iii) $-x_1, x_2, -x_3+3/2, x_4$; (iv) $x_1-1/2, -x_2+1/2, -x_3+1, -x_4$; (v) $-x_1, -x_2, -x_3+1, -x_4$; (vi) $x_1, -x_2, x_3+1/2, -x_4$.