Structural phase transition and related electronic properties in quasi one-dimensional $(NbSe_4)_{10/3}I$

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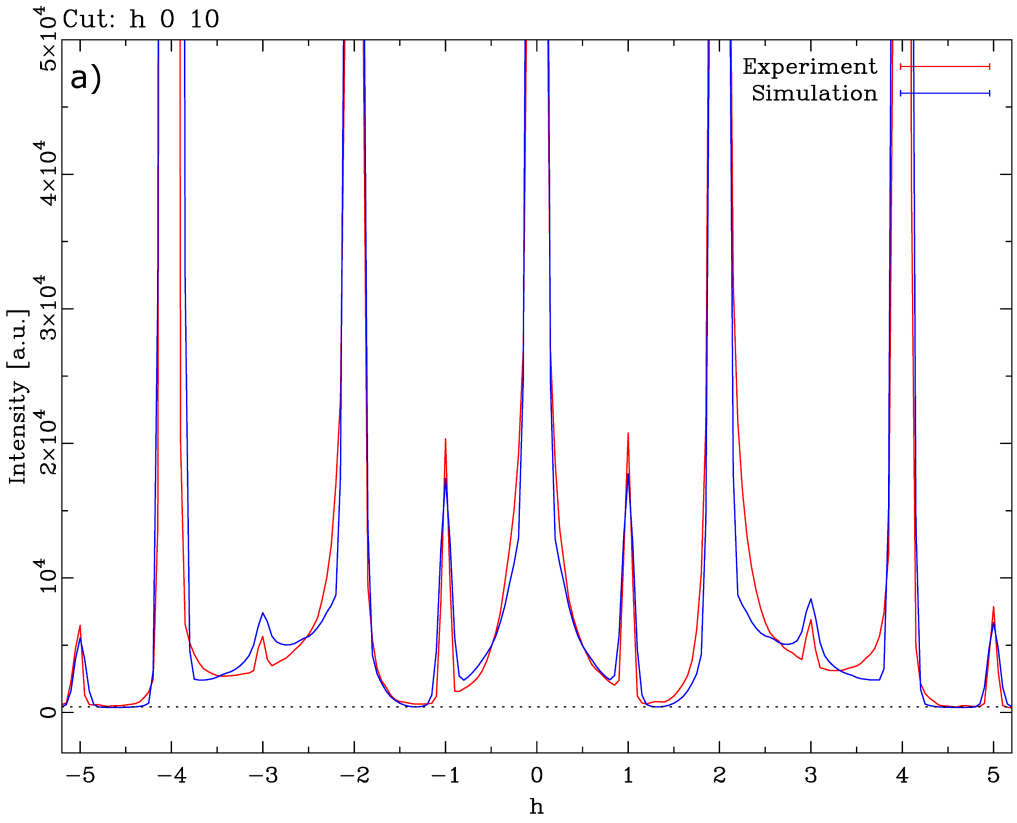
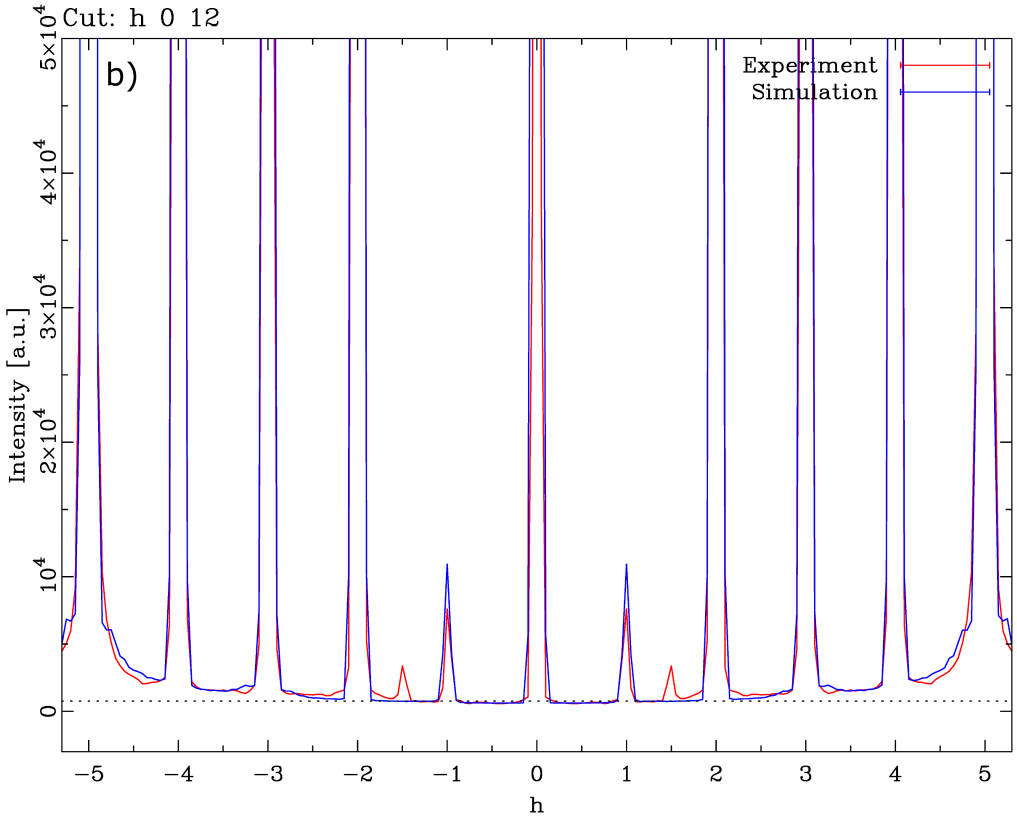
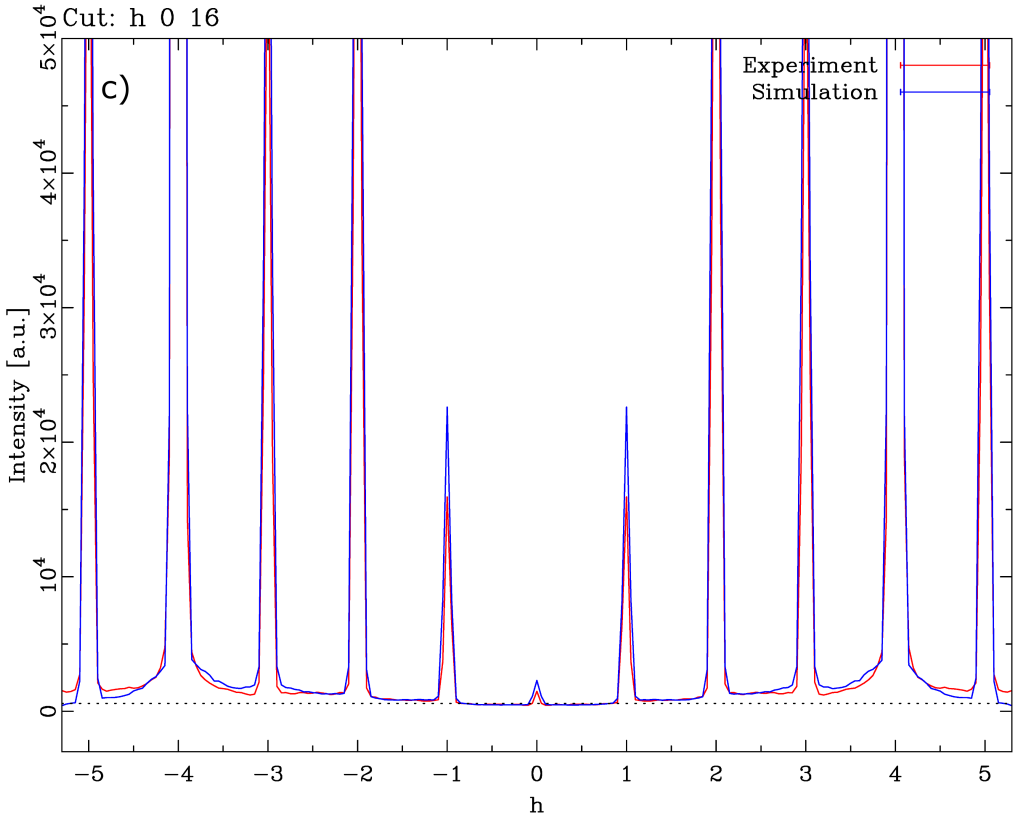
Supplementary material




Cut: h 0 12
b)
Experiment
Simulation
Intensity [a.u.]
0
10^4
2×10^4
3×10^4
4×10^4
5×10^4
−5
−4
−3
−2
−1
0
1
2
3
4
5
h


Cut: h 0 16
c)
Experiment
Simulation
Intensity [a.u.]
0
10^4
2×10^4
3×10^4
4×10^4
5×10^4
−5
−4
−3
−2
−1
0
1
2
3
4
5
h

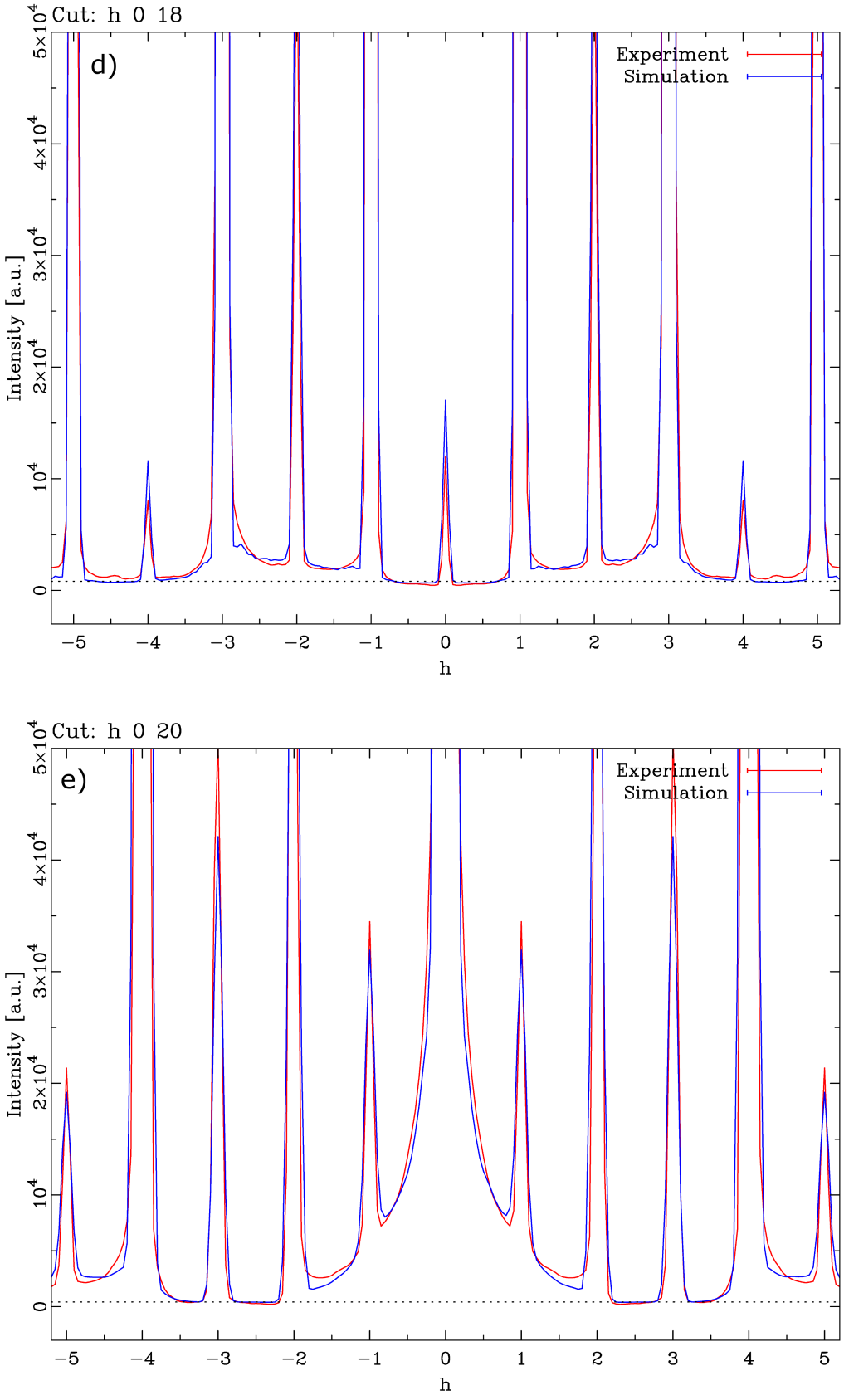

Cut: h 0 18
d)
Experiment
Simulation
Intensity [a.u.]
h
Cut: h 0 20
e)
Experiment
Simulation
Intensity [a.u.]
h

Figure S1

Comparison of one-dimensional sections through the diffuse scattering, stretched perpendicular to the ***c**** direction and with common intersections with the hk planes, at selected points in the reciprocal space: (a) (h 0 10), (b) (h 0 12), (c) (h 0 16) , (d) (h 0 18) and (e) (h 0 20).

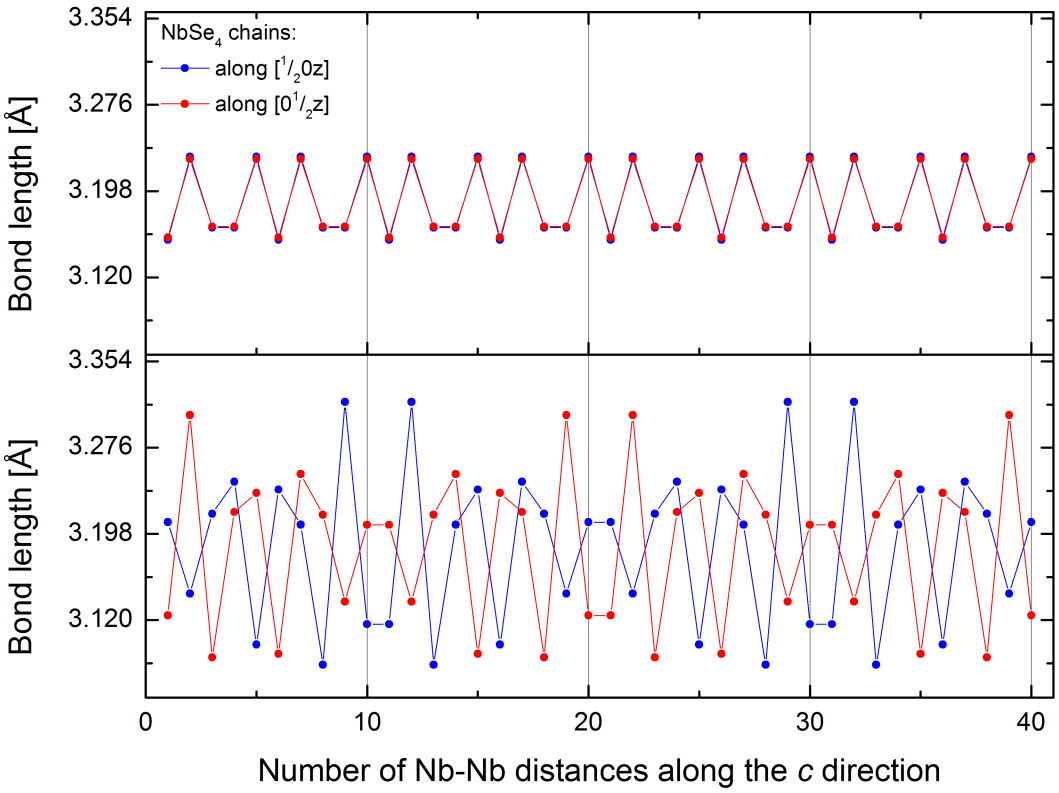


Figure S2

Nb-Nb distances at 100 K in the average structure (upper part) and in the superstructure approximation (bottom part) with two different chains present in the superstructure cell. Two superstructure and four average structure cells are shown. Vertical lines represent periods of the average unit cell along *c* direction.

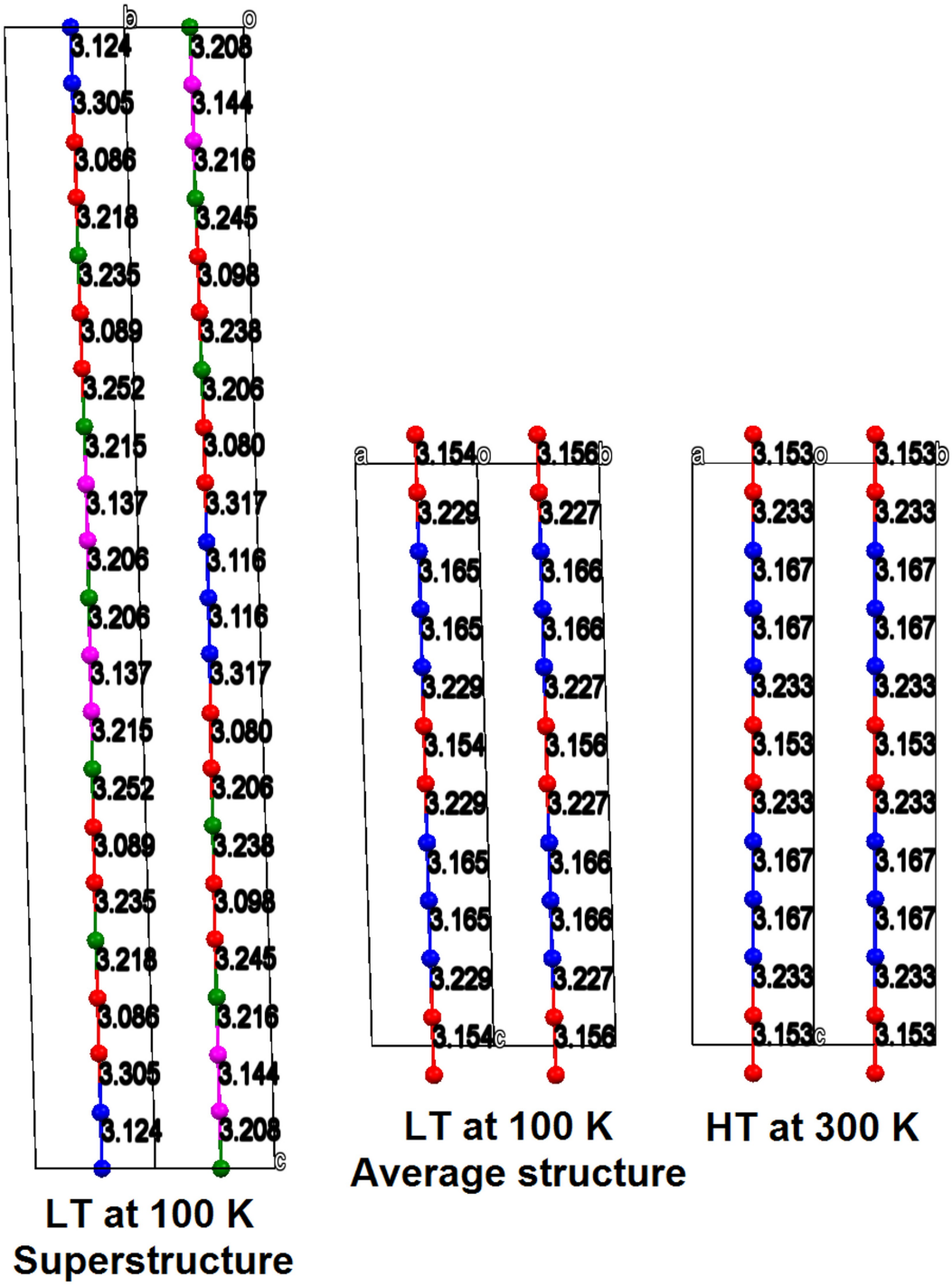


Figure S3

Comparison of the Nb-Nb distances in the HT (300 K) and LT (100 K) average structures and in the superstructure approximation at 100 K. Only Nb atoms are shown. Green are isolated Nb atoms with large distances to the neighbouring atoms, red and magenta are Nb_2 pairs with shortest and intermediate distances, and blue are Nb_3 groups with intermediate distances.