Comment about :

Condensed Matter Physics, 2013, Vol. 16, No 1, 13602: 1–8
DOI: 10.5488/CMP.16.13602
Title : Study of the validity of a combined potential model using the hybrid reverse Monte Carlo method in fluoride glass system
Authors : S.M. Mesli, M. Habchi, M. Kotbi, H. Xu

In this paper I could recognize the figure 1 as being taken from the figures 6 and 7 of my own work cited in reference [10] :
https://arxiv.org/ftp/cond-mat/papers/0310/0310487.pdf
Title : Reverse Monte Carlo and Rietveld modelling of BaMn(Fe,V)F7 glass structures from neutron data
Author : Armel Le Bail
Proceedings of CONCIM 2003 - Conference on Non-Crystalline Inorganic Materials - April 8-12, 2003, Bonn, Germany.

Comparison of Mesli figure 1 and of my figures 6 and 7 :

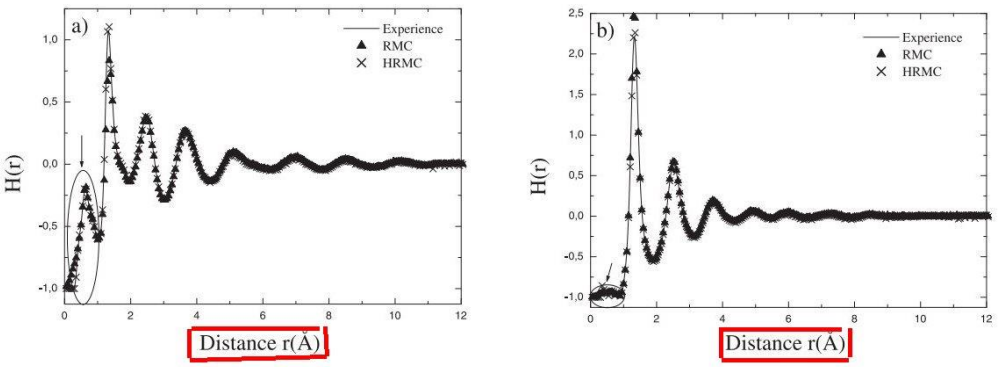

Figure 1. HRMC, RMC and experimental data: total distribution function $G(r)$ of (a) $BaMnFeF_7$ and (b) $BaMnVF_7$ at the glassy state; total correlation functions are represented $H(r) = G(r) - 1$.

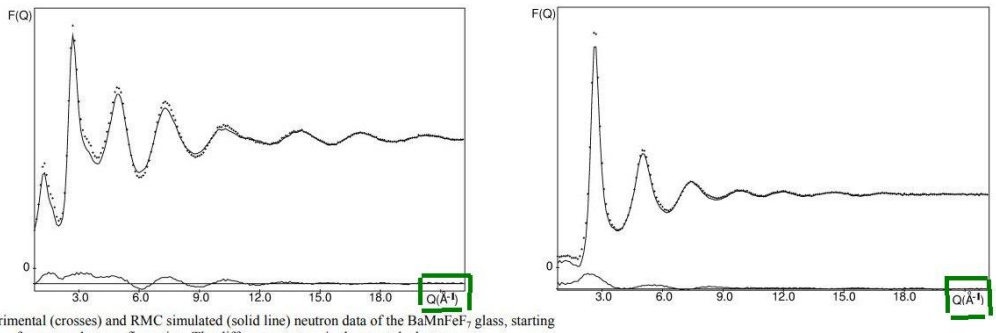

Fig. 6 - Experimental (crosses) and RMC simulated (solid line) neutron data of the $BaMnFeF_7$ glass, starting from a random configuration. The difference pattern is shown at the bottom.

Fig. 7 - Experimental (crosses) and RMC simulated (solid line) neutron data of the $BaMnVF_7$ glass, starting from a random configuration. The difference pattern is shown at the bottom.

Mesli et al. are more or less saying that they have taken my data. But the problem being here that my figures 6 and 7 are the original neutron diffraction data of two fluoride glasses and the scale is given in Q(angstrom-1), they are so-called structure factor curves, whereas the figure 1 in the Mesli et al. paper shows the same curves after a change of the Q scale into a R(angstrom) scale and they are renamed radial distribution functions. This is an obvious falsification.

The only way to produce a radial distribution function from a structure factor curve is to apply a Fourier transformation and then the obtained curve cannot be the same as the original one.

It is thus obvious here that the paper from Mesli et al. is in consequence fake. The data are falsified by an arbitrary change of Q scale into R scale. All the calculations based on these fake radial distribution functions are complete non-sense. By the way, the same fake radial distribution functions are in the Mesli PhD thesis as fig 4.3 :

4.3.2 Résultats et discussions

Les fonctions de corrélation totales $H(r)$

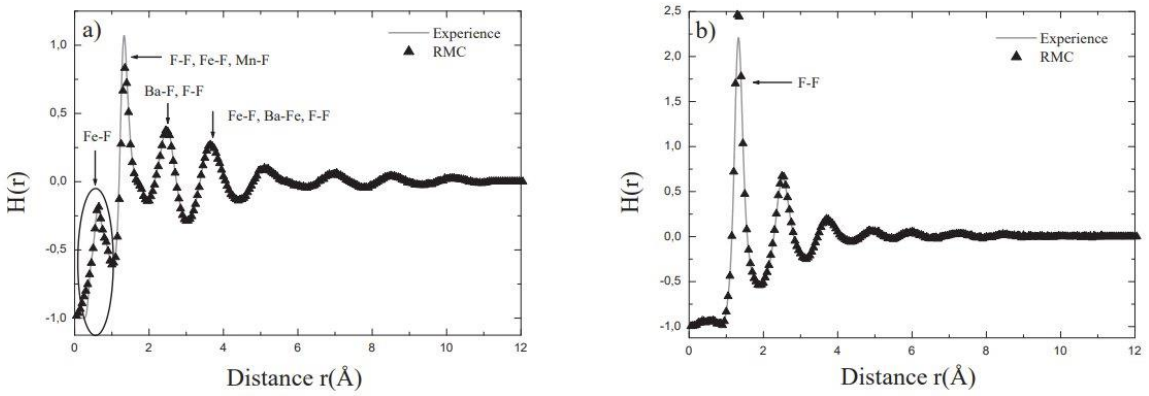

FIGURE 4.3 – Comparaison des résultats expérimentaux à celles de la simulation RMC, des fonctions de corrélations totales $H(r)$: (a) $BaMnFeF_7$ et (b) $BaMnVF_7$

Link to the Mesli thesis :
http://dspace.univ-tlemcen.dz/bitstream/112/4181/1/these_finale_mesli-1.pdf

That time, the figure 4.3 above is annotated with an interpretation of the peaks as corresponding to interatomic distances in the fluoride glasses. For instances Fe-F distances < 1 angstrom and F-F distances < 2 angtroms. Such interatomic distances are simply impossible.

The true radial distribution functions for these glasses were calculated by me and shown in my own PhD thesis in 1985, page 79, figure 23 :

http://www.cristal.org/CHM/Doctorat-Etat-Le-Bail-A.pdf

The results confirmed classical Fe-F distances of 1.93 angstroms.

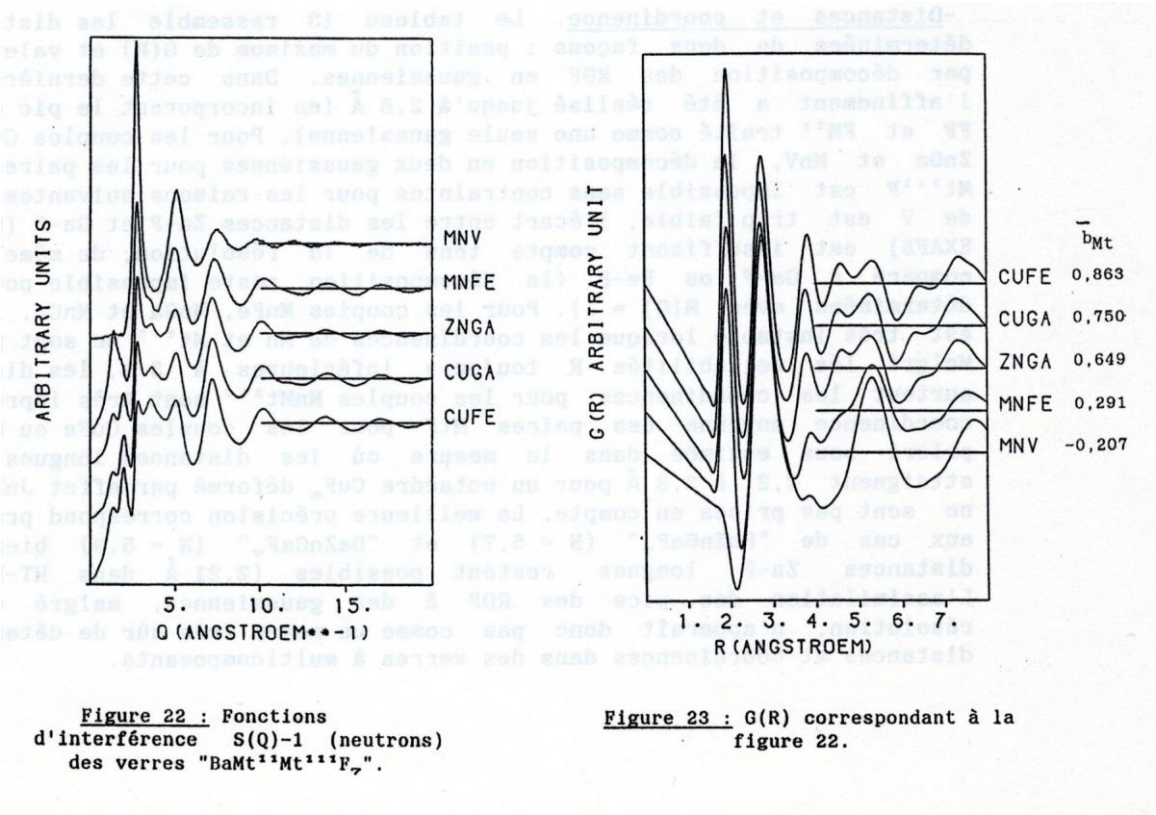

Figure 22 : Fonctions d'interférence S(Q)-1 (neutrons) des verres "$BaMt^{II}Mt^{III}F_7$".

Figure 23 : G(R) correspondant à la figure 22.

The figure 22 in my own 1985 PhD thesis shows the neutron interference functions for a series of fluoride glasses including BaMnFeF7 and BaMnVF7 and the Fourier transforms providing the radial distribution functions are shown on figure 23 on the right.

So, Mesli et al., since they pretend to show on their Figure 1 the radial distribution functions, they should have copied my figure 23 instead of the above figure 22. Consequently their radial distribution functions are fake. Any RMC (Reverse Monte Carlo) modelling from fake radial distribution functions will produce fake results.

CONCLUSION

We are in presence of a strong misconduct. The full Mesli thesis is based on the falsification of two figures leading to impossible interatomic distances. These fake results are reproduced into several published paper which have to be retracted, as well as the thesis. How the thesis director and the jury members could not see that such Fe-F distances being less that 1 angstrom was impossible is quite of a mystery.

Additional links :

Comments at PubPeer :
https://pubpeer.com/publications/3837C565C836A452AC77BAF98B30F1
https://pubpeer.com/publications/501B561FF3980FC69C34B9A8B80CCE
See also the discussion of that case in the CHM (Crystallography Horror Museum) :
http://www.cristal.org/CHM/CHM.html#18

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