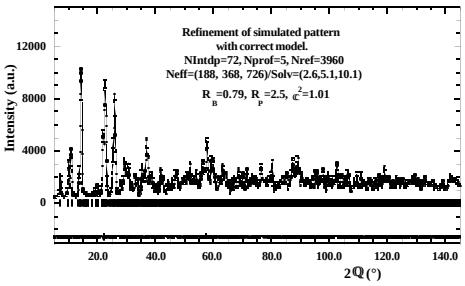
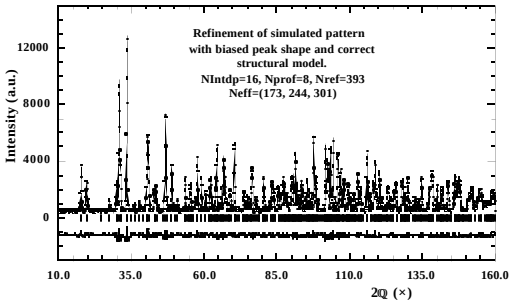
Results of simulations: Refinements of simulated powder diffraction patterns using correct and biased models

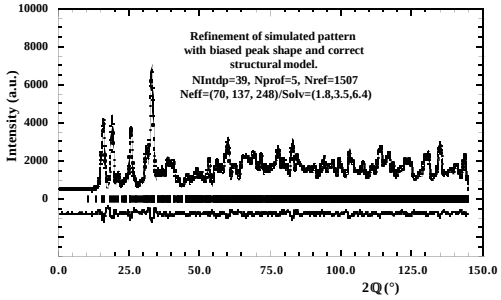
RM (systematic errors): Correct structural and peak shape model N_I=72 (Plot-pattern)



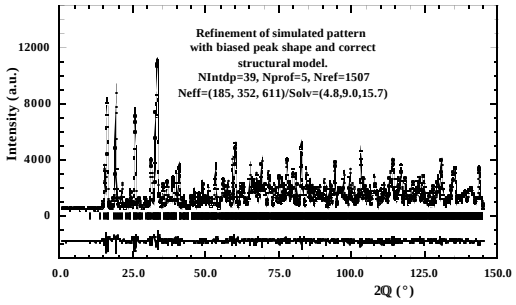
RM (systematic errors): Correct structural model, biased peak shape N_I=16 (Plot-pattern)



RM (systematic errors): Biased peak shape+ correct structural model N_I=39 + bad resolution

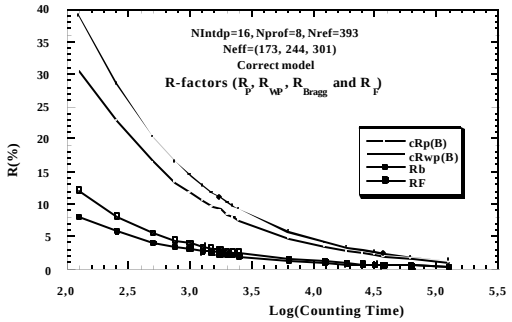


RM (systematic errors): Biased peak shape+ correct structural model N_I=39 + better resolution

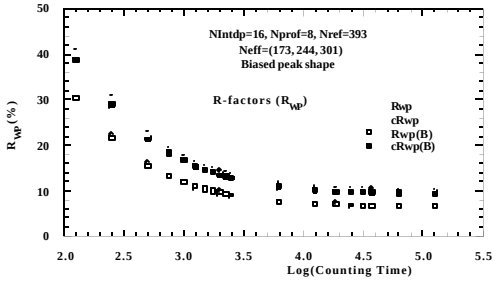


Behaviour of Rietveld R-factors, and other indicators, versus counting statistics for perfect and biased models

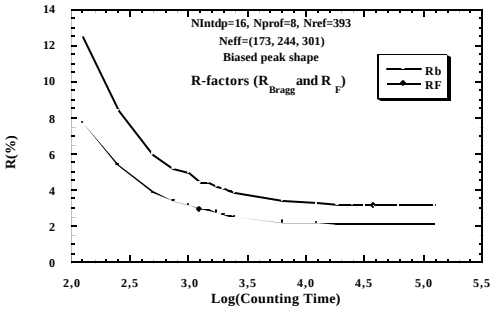
RM (systematic errors): Behaviour of R-factors versus counting time (correct model)



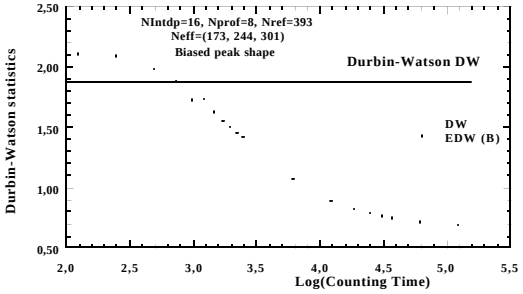
RM (systematic errors): Behaviour of R_{WP} factors versus counting time (biased peak shape)



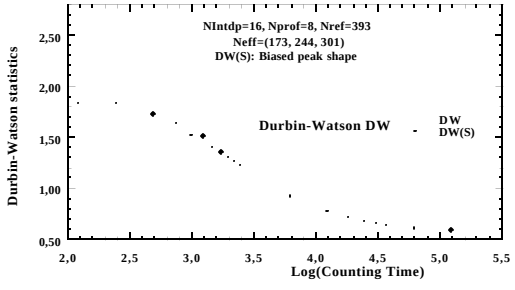
RM (systematic errors): Behaviour of R_{Bragg} and R_F factors versus counting time (biased peak shape)



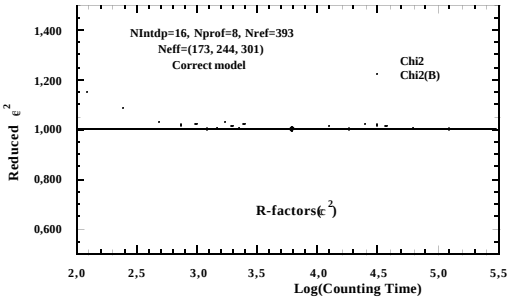
RM (systematic errors): Behaviour of DW indicators versus counting time (biased peak shape)



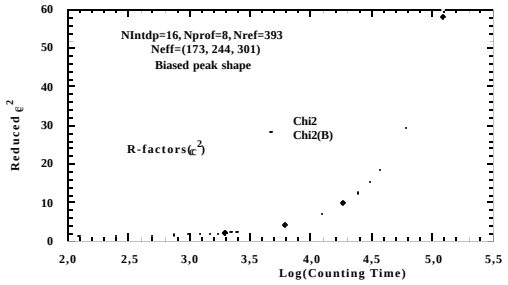
RM (systematic errors): Behaviour of DW indicator versus counting time (biased/unbiased peak shape)



RM (systematic errors): Behaviour of reduced Chi-square versus counting time (correct model)

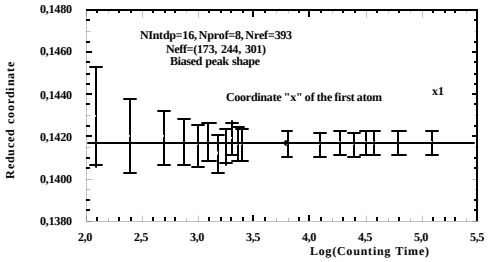


RM (systematic errors): Behaviour of reduced Chi-square versus counting time (biased peak shape)



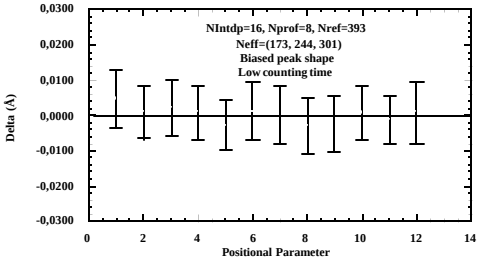
Behaviour of positional parameters (atom co-ordinates), versus counting statistics, resolution, ... for perfect and biased models

RM (systematic errors): Behaviour of positional parameters versus counting time (biased peak shape)

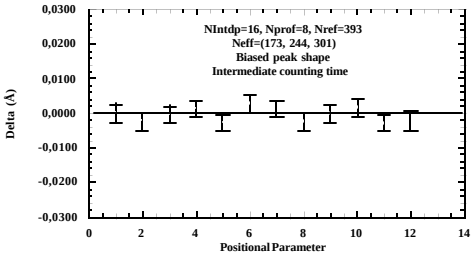


Atom co-ordinates versus counting statistics

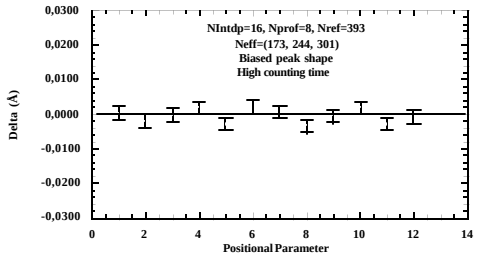
RM (systematic errors): Positional parameters N_I=16, Low counting time (biased peak shape)



RM (systematic errors): Positional parameters, N_I=16 Intermediate counting time (biased peak shape)

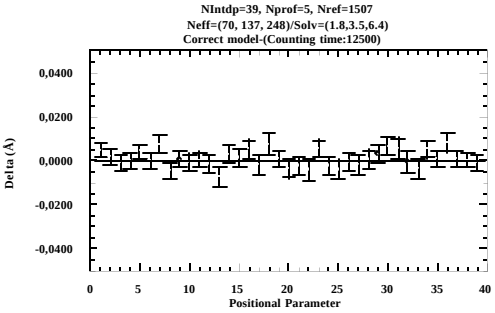


RM (systematic errors): Positional parameters, N_I=16
High counting time (biased peak shape)

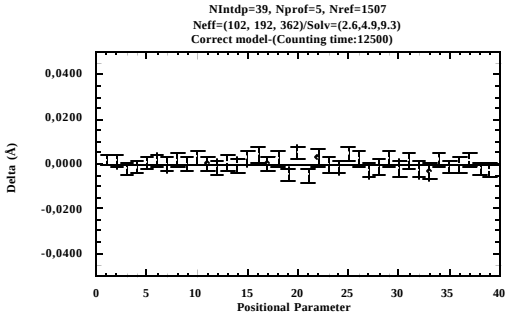


Atom co-ordinates versus resolution ("solvability index")
$r=N_{eff}/N_I$

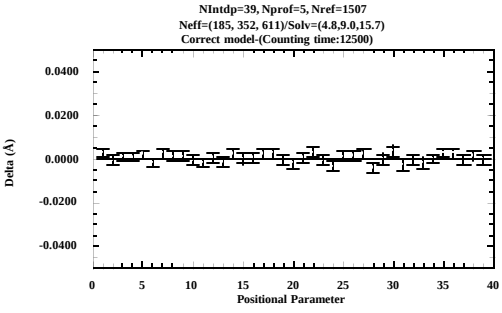
RM (systematic errors): Positional parameters
N_I=39, Counting Time: 12500 (correct model, r=3.5)



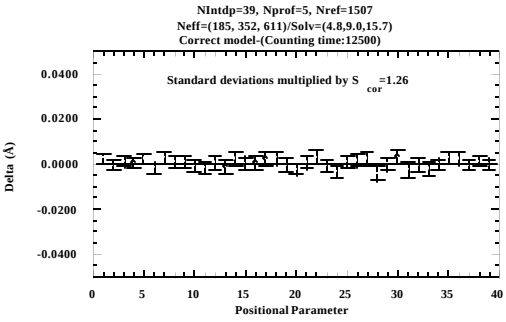
RM (systematic errors): Positional parameters
N_I=39, Counting Time: 12500 (correct model, r=4.9)



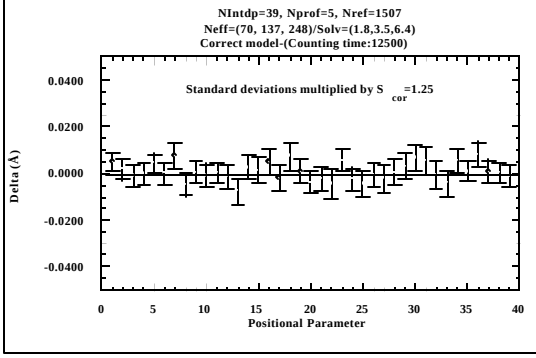
RM (systematic errors): Positional parameters
N_I=39, Counting Time: 12500 (correct model, r=9)



RM (systematic errors): Positional parameters
N_I=39, Counting Time: 12500 (correct model, r=9, Sx)

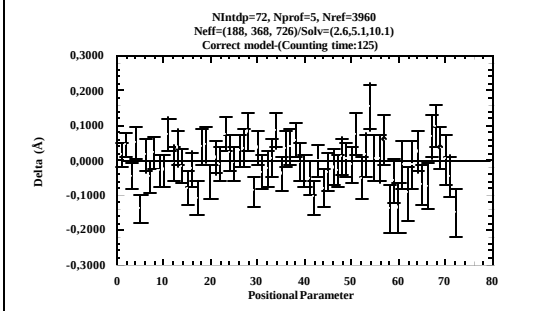


RM (systematic errors): Positional parameters
N_I=39, Counting Time: 12500 (correct model, r=3.5, Sx)

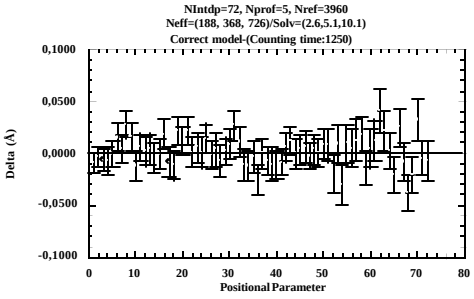


Atom co-ordinates versus statistics (correct model, N_I=72)

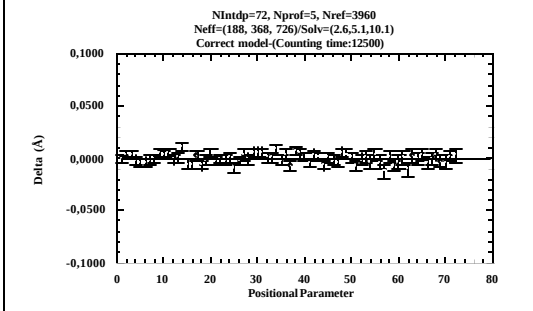
RM (systematic errors): Positional parameters
N_I=72, Counting Time: 125 (correct model, r=5.1)



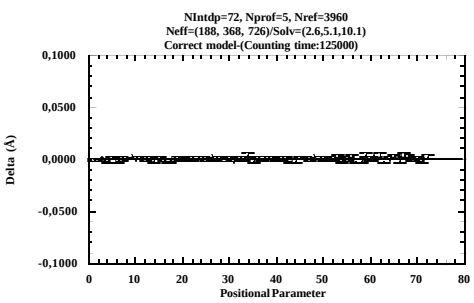
RM (systematic errors): Positional parameters
N_I=72, Counting Time: 1250 (correct model, r=5.1)



RM (systematic errors): Positional parameters
N_I=72, Counting Time: 12500 (correct model, r=5.1)

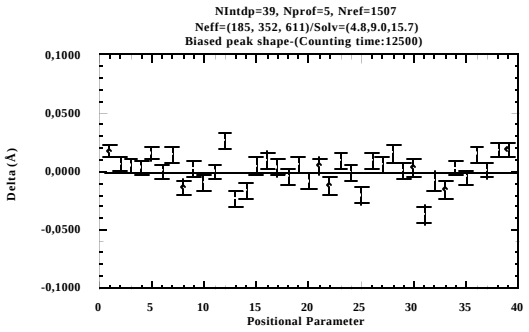


RM (systematic errors): Positional parameters
N_I=72, Counting Time: 125000 (correct model, r=5.1)

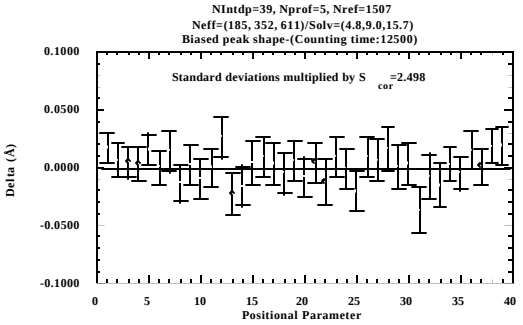


Atom co-ordinates versus statistics
(biased peak shape, N_I=39)

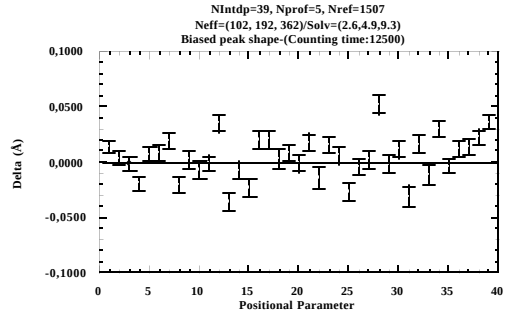
RM (systematic errors): Positional parameters
N_I=39, Counting Time: 12500 (biased peak shape, r=9)



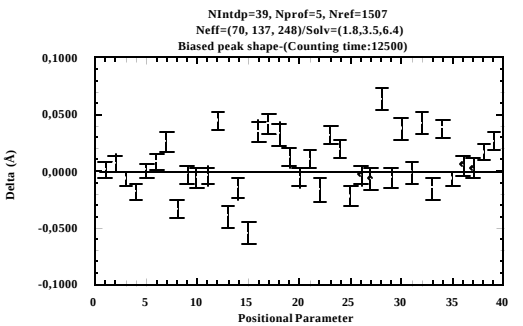
RM (systematic errors): Positional parameters
N_I=39, Counting Time: 12500 (biased peak shape, r=9, Sx)



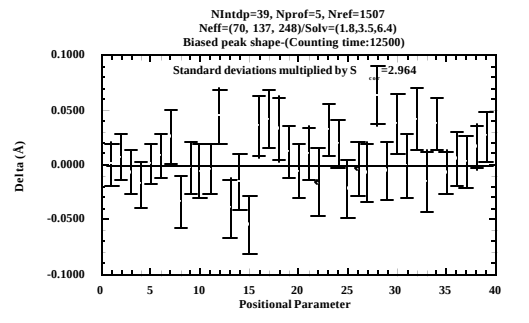
RM (systematic errors): Positional parameters
N_I=39, Counting Time: 12500 (biased peak shape, r=4.9)



RM (systematic errors): Positional parameters
N_I=39, Counting Time: 12500 (biased peak shape, r=3.5)

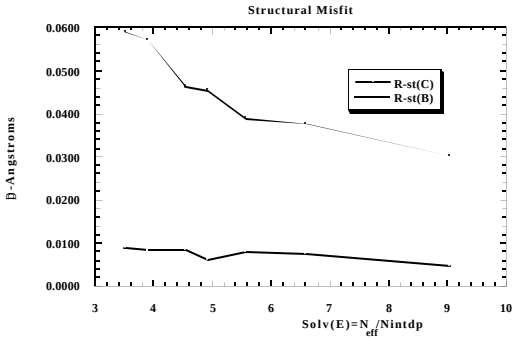


RM (systematic errors): Positional parameters
N_I=39, Counting Time: 12500 (biased peak shape, r=3.5, Sx)



Structural misfit versus resolution

RM (systematic errors): Structural misfit versus N_{eff}/N_I



RM (systematic errors): Structural misfit versus N_{eff}/N_I