```
TITLE
NI(OH)2 WITH DEFORMATION AND GROWTH FAULTS

Instrumental  And  Size  Broadening
!Type Of Radiation
 Radiation      X-Ray
!               lambda1    lambda2   ratio
 Wavelength      1.5406    0.0000    0.0000
!instrumental aberrations      zero      sycos     sysin
 Aberrations                  0.0000    0.0000    0.0000
                                0.00      0.00      0.00
!instr. broadening       u           v           w           x         Dg         Dl
 Pseudo-Voigt       0.032948   -0.003558    0.227400    0.000000     479.26     459.87 Trim
                       1.00        0.00        0.00        0.00       1.00       1.00

 Structural
 !         a            b            c          gamma
 Cell      3.128608    3.128608    4.608609     120.00
             21.00       21.00        1.00       0.00
!Laue symmetry
 Symm  -3M
!number of layer types
 Nlayers   4
!layer width
 Lwidth  Infinite

 Layer 1
!Layer symmetry
 LSYM   CentroSymmetric
!Atom name   number   x         y         z         Biso      Occ
 Atom Ni2+        1   0.67000   0.33000   0.00000   1.06197   0.50000
                      0.00      0.00      0.00      0.00      0.00
!Atom name   number   x         y         z         Biso      Occ
 Atom O2-         2   0.33000   0.67000   0.22265   0.75961   1.00000
                      0.00      0.00     71.00      0.00      0.00

 Layer 2 = 1

 Layer 3 = 1

 Layer 4
!Layer symmetry
 Lsym   Centrosymmetric
!Atom name   number   x         y         z         Biso      Occ
 Atom Ni2+        3   0.00000   0.00000   0.00000   1.06197   0.50000
                      0.00      0.00      0.00      0.00      0.00
!Atom name   number   x         y         z         Biso      Occ
 Atom O2-         4   0.33000   0.67000   0.22265   0.75961   1.00000
                      0.00      0.00     71.00      0.00      0.00

 Stacking
!stacking type
 Recursive
!number of layers
  40.0
  1.0

 Transitions

!layer  1 to layer  1
Lt   0.808196  0.000000  0.000000  1.000000
   -92.000000  0.000000  0.000000  0.000000
Fw       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  1 to layer  2
LT   0.095902  0.333000  0.666700  1.000000
    91.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  1 to layer  3
LT   0.000000  0.000000  0.000000  0.000000
     0.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  1 to layer  4
LT   0.095902  0.000000  0.000000  1.000000
    91.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00


!layer  2 to layer  1
LT   0.000000  0.000000  0.000000  0.000000
     0.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  2 to layer  2
LT   0.919278  0.000000  0.000000  1.000000
  -101.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  2 to layer  3
LT   0.080722  0.333000  0.666700  1.000000
   101.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  2 to layer  4
LT   0.000000  0.000000  0.000000  0.000000
     0.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
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!layer  3 to layer  1
LT   0.132589  0.333000  0.666700  1.000000
  -111.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  3 to layer  2
LT   0.000000  0.000000  0.000000  0.000000
     0.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  3 to layer  3
LT   0.867411  0.000000  0.000000  1.000000
   111.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  3 to layer  4
LT   0.000000  0.000000  0.000000  1.000000
     0.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00


!layer  4 to layer  1
LT   0.108204  0.000000  0.000000  1.000000
   -41.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  4 to layer  2
LT   0.000000  0.000000  0.000000  1.000000
     0.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  4 to layer  3
LT   0.000000  0.000000  0.000000  0.000000
     0.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00
!layer  4 to layer  4
LT   0.891796  0.000000  0.000000  1.000000
    41.000000  0.000000  0.000000  0.000000
FW       0.00      0.00      0.00      0.00      0.00      0.00
         0.00      0.00      0.00      0.00      0.00      0.00

 Calculation
 Lmq
 Corrmax      30
 Maxfun     2400
 Tol       0.100000E-04
 Nprint       0

 Experimental
!Filename                    Scale factor     code
 FILE  cer+simul.dat                0.812         1.00
 Excluded_Regions   2
    0.0000    8.0000
  135.0000  180.0000
 FFORMAT  free
!Linear interpolation
 Bgrinter    Sim.Bgr
!Polynomial  Number of coefficients
 Bgrcheb           2
!Polynomial coefficients
     1.00000     0.20000
     1.0         1.0
!number of pattern backgrounds
 Bgrnum  1
!Pattern file           Filename      Scale factor     code
 Bgrpatt           cerusite1.sub        0.026000       1.00   cerusite.hkl
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