# EXAFS by itself and in good company

**Victor Krayzman**
(NIST)

EXAFS-50 Symposium

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# EXAFS spectroscopy: a new method for structural investigation

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Usp. Fiz. Nauk **149**, 275–324 (June 1986)

EXAFS spectroscopy is a new method of investigating materials which allows one to determine structural parameters of the local environment of atoms with some specified $Z$ by studying their x-ray spectra. Among these parameters are the interatomic spacings, coordination numbers and amplitudes of thermal oscillations. It is not necessary for long-range order to be present in the sample under investigation. Depending on the way this technique for obtaining the spectrum is applied, one can analyze the local environment of atoms located either within the sample volume or at its surface. We investigate the physical phenomena on which the method is based, the mathematical techniques used to process the experimental data, and various methods of recording the spectra. We present a series of examples in which EXAFS spectroscopy is used to study superionic conductors, compounds with intermediate valence, biological molecules, solid solutions, catalysts, surface layers and intercalated compounds.

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*J. Synchrotron Rad.* (1999). **6**, 158–160

# Laboratory diffractometer-based XAFS spectrometer

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The device has been developed to allow XAFS spectra of good quality to be obtained using conventional powder diffractometer. The device is based on the mechanical system which synchronize the changes of curvature radius of bent crystal-monochromator with the Bragg angle. Due to high resolution (1-10 eV depending on the wavelength) and photon flux only several hours are needed to perform quality XAFS experiment. The device is easy to operate and can be successfully used both for XAFS investigations and for student's practice.

**Keywords: XAFS spectrometer, XAFS laboratory experimental facilities**

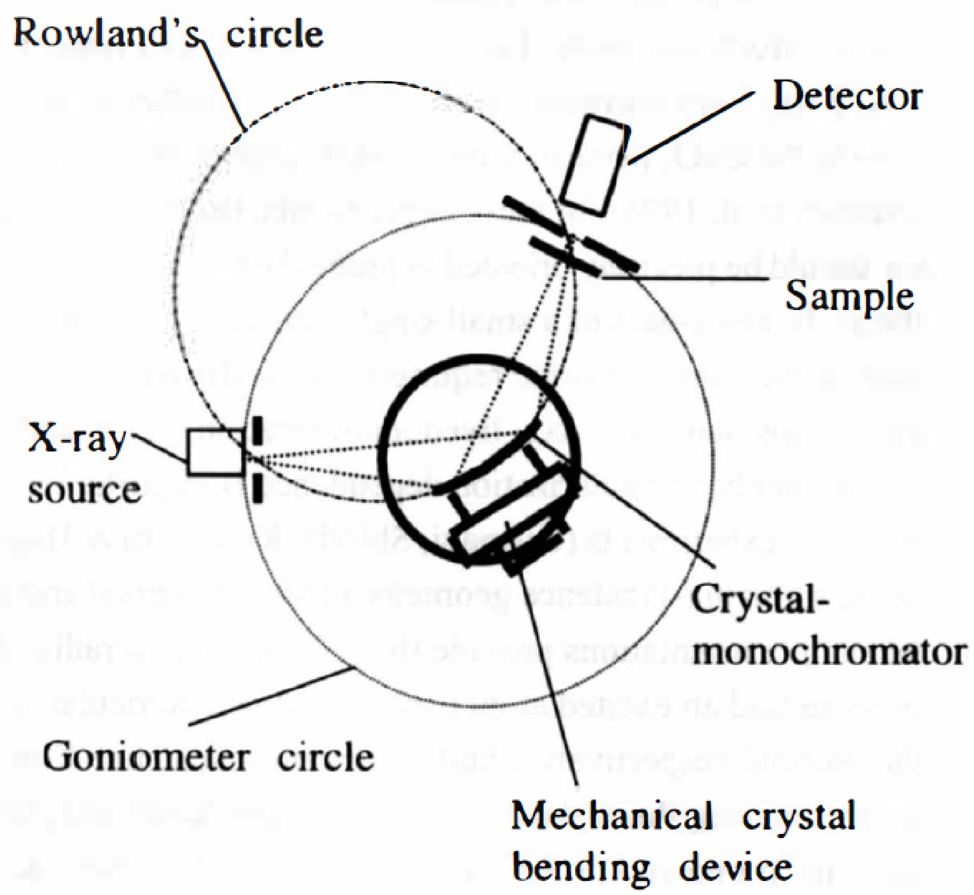


**Figure 1**
Schematic view of the laboratory diffractometer- based XAFS spectrometer

## EXAFS study of graphite intercalation compound with transition metals (Fe,Ni)

Shuvaev A.T. , Khelmer B.Y., Lyubeznova T.A., Kraizman V.L., Mirmilstein A.S., Kvacheva L.D., Novikov Yu. N. and Volpin M. E.

J. Phys. France **50,** 1145 (1989)

## Study of dynamics of iron trichloride hydration and oxidation by the x-ray absorption-spectroscopy technique.

Shuvaev A.T. , Khelmer B.Y., Lyubeznova T.A., Kraizman V.L., Novakovich A.A.

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Phys. Stat. Sol. B **105**, 747 (1981)

$$\chi_K^{(\alpha)}(k) = -4\pi\rho \sum_{\beta} c_\beta \frac{\left|f_\beta(k,\pi)\right| Z_K^{(\alpha)}}{k} \int_0^\infty g_{\alpha\beta}(R) e^{-\frac{2R}{\lambda}} \sin\left(2kR + 2\delta_1^{(\alpha)} + \vartheta_\beta\right) dR$$

$$N_{\alpha\beta}(R_1, R_2) = 4\pi\rho c_\beta \int_{R_1}^{R_2} r^2\, g_{\alpha\beta}(r) dr$$

$$I(s) = 1 + \frac{4\pi\rho}{sF_0^2(s)} \sum_{\alpha}\sum_{\beta} c_\alpha F_\alpha(s)\, c_\beta F_\beta(s) \int_0^\infty \left(g_{\alpha\beta}(r) - 1\right) \sin(sr) r dr$$

$$s = 4\pi \sin(\theta)/\lambda$$

# Reverse Monte Carlo

## RMCProfile software package

Data sets for powder samples

1. Neutron total scattering in R space and in Q space
2. X-ray total scattering in R space and in Q space
3. Bragg profile
4. EXAFS

Electron, X-ray, and neutron diffuse scattering for single crystals

Metropolis algorithm for minimization of total residual $R = \sum w_i R_i$

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# A combined fit of total scattering and extended X-ray absorption fine structure data for local-structure determination in crystalline materials

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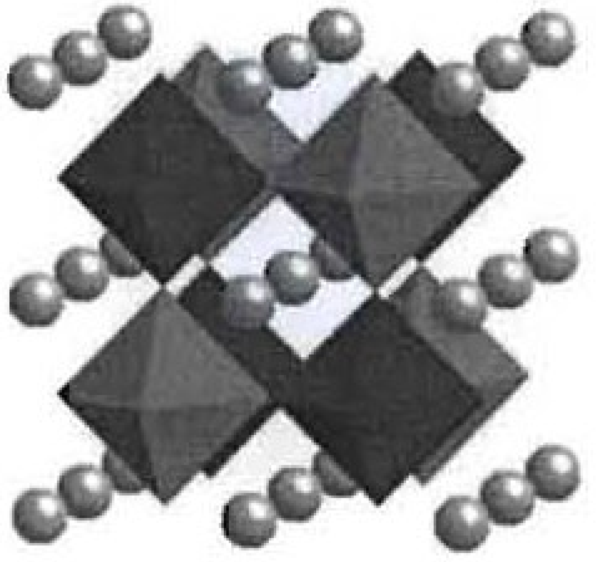


$SrAl_{1/2}Nb_{1/2}O_3$ structure

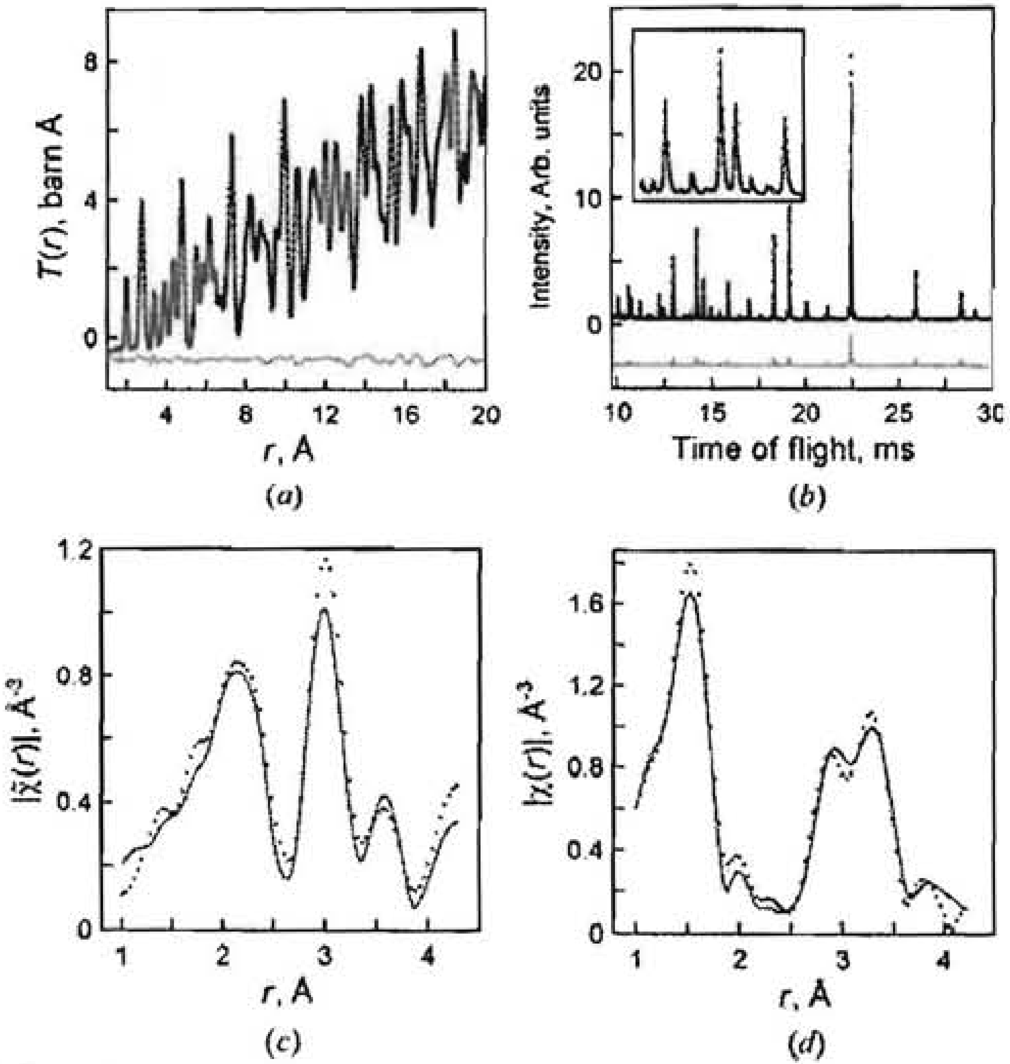
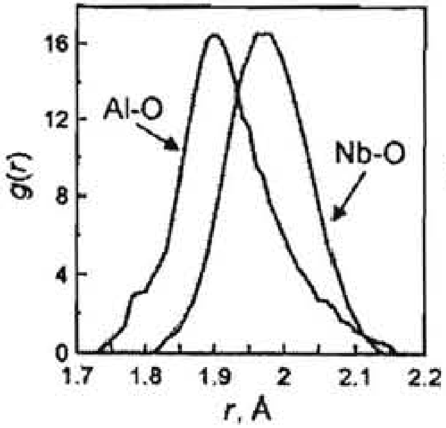



**Figure 4**
Experimental (dotted lines) and calculated (solid lines) (*a*) $T(r)$, (*b*) Bragg, and (*c*) Sr EXAFS and (*d*) Nb EXAFS profiles for $SrAl_{1/2}Nb_{1/2}O_3$ obtained by a simultaneous RMC fit. The inset in (*b*) displays a magnified view of the high-$Q$ range of the Bragg profile. The $k$ ranges used in EXAFS Fourier transforms were 3.3–13.2 $Å^{-1}$ for Nb and 3.0–14.2 $Å^{-1}$ for Sr.



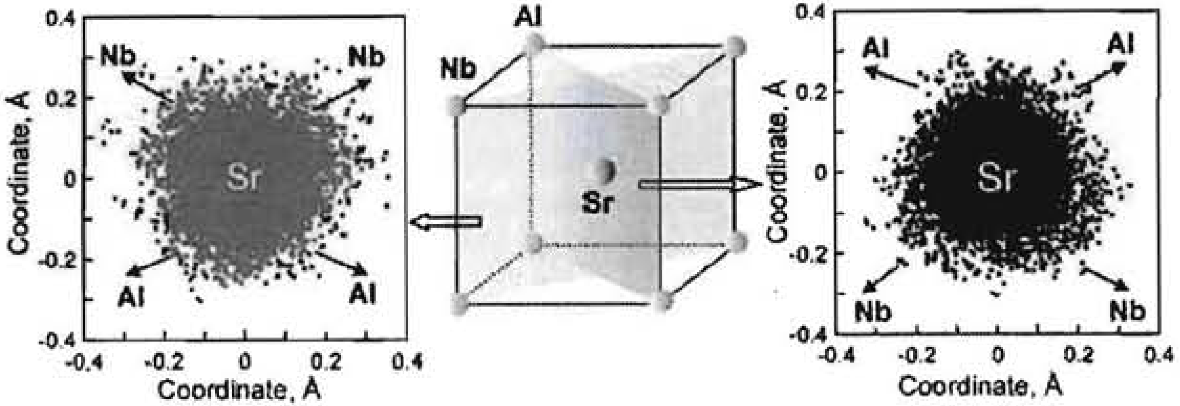




**Figure 10**
(Middle) Schematic drawing of the Sr coordination by Nb and Al in SAN. (Left, right) Projections of the Sr probability density function on the [110] and [1$\bar{1}$0] sections, respectively. Each point in these plots represents an instantaneous Sr position. Arrows indicate the directions toward the neighboring *B* cations. A pronounced complementary asymmetry of the two sections is observed.

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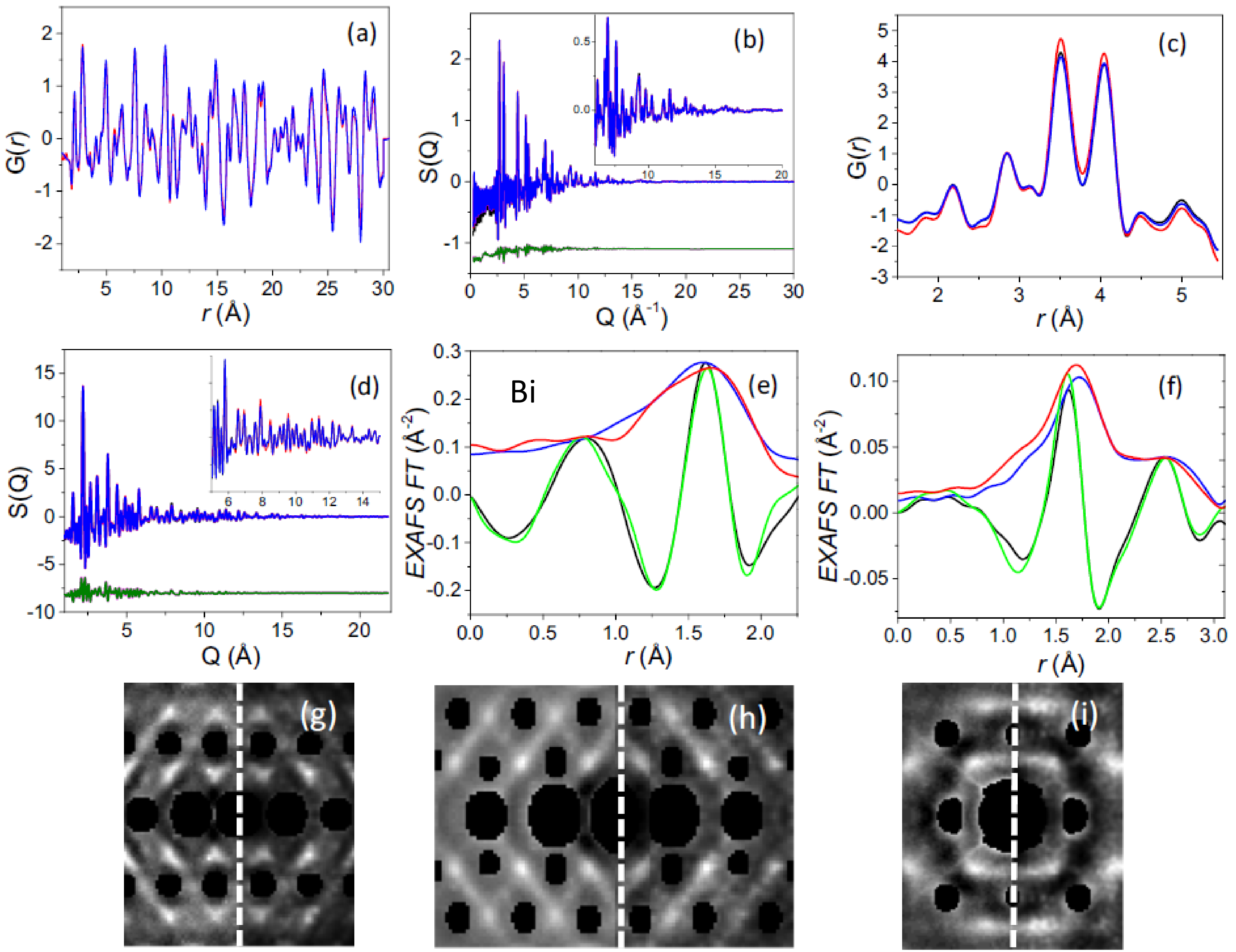
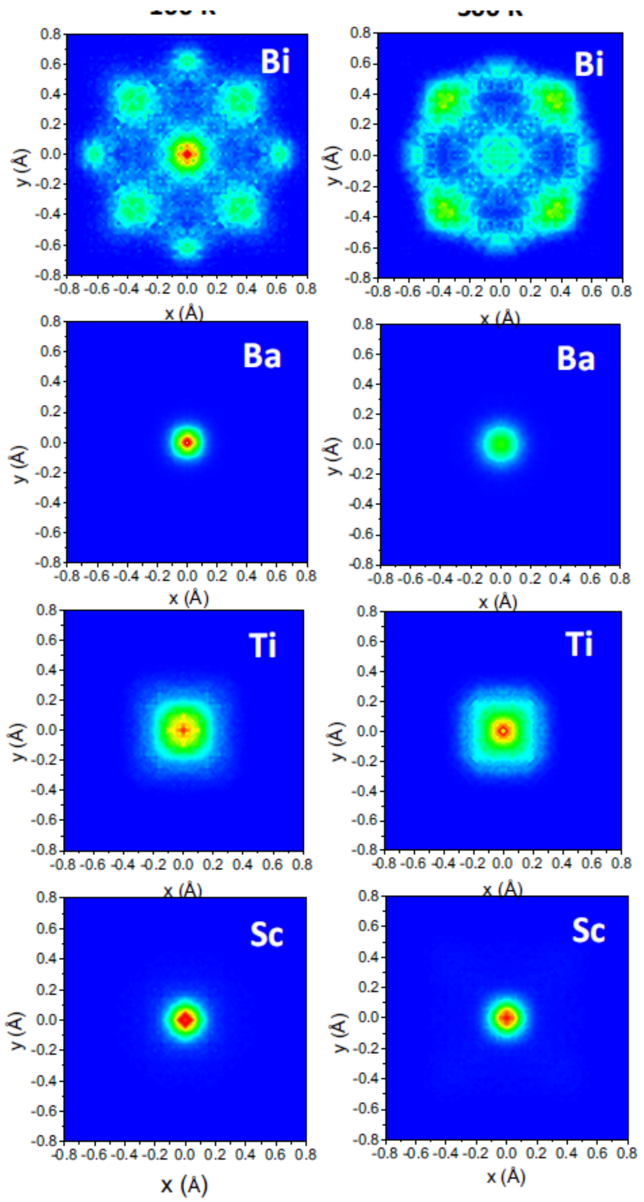
# Local structure in $BaTiO_3$-$BiScO_3$ dipole glasses

I. Levin, V. Krayzman, J. C. Woicik, F. Bridges,
G. E. Sterbinsky, T-M. Usher, J. L. Jones, and D. Torrejon

$(Ba_{0.6}Bi_{0.4})(Ti_{0.6}Sc_{0.4})O_3$ solid solutions



(a)
G(r)
r (Å)
(b)
S(Q)
Q (Å$^{-1}$)
(c)
G(r)
r (Å)
(d)
S(Q)
Q (Å)
(e)
Bi
EXAFS FT (Å$^{-2}$)
r (Å)
(f)
EXAFS FT (Å$^{-2}$)
r (Å)
(g)
(h)
(i)



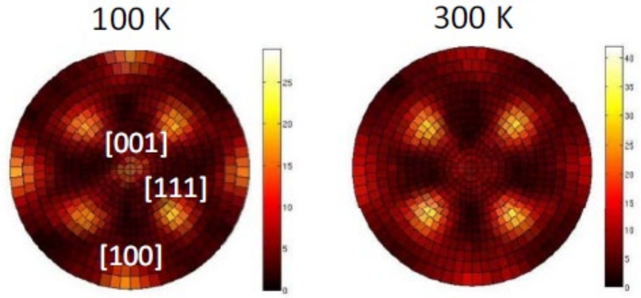




FIG. 16. Stereographic projections displaying the PDDs for directions of the Bi displacements at 100 K and 300 K. These distributions exhibit well-defined maxima for the ⟨111⟩ and ⟨100⟩ directions. The relative probability of ⟨111⟩ displacements is larger at 300 K.

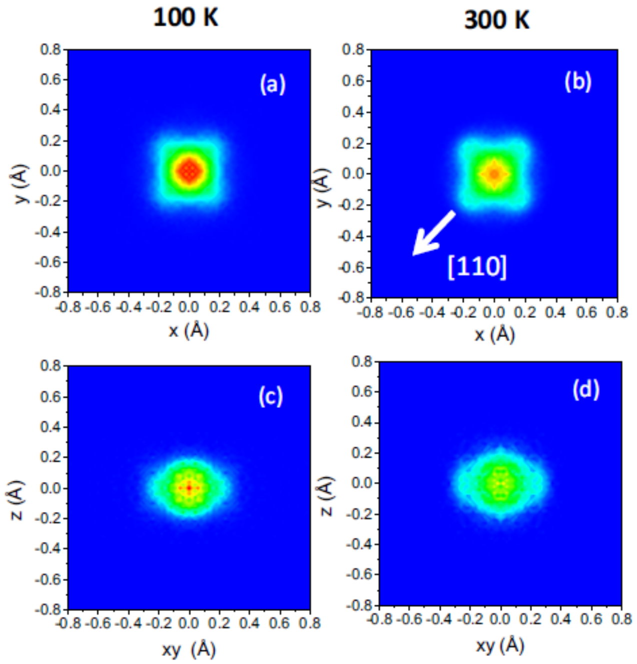



FIG. 17. (a–b) PDDs of oxygen atoms projected onto {001} plane; (c–d) a {110} slice through this PDD.

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# Local atomic order and hierarchical polar nanoregions in a classical relaxor ferroelectric

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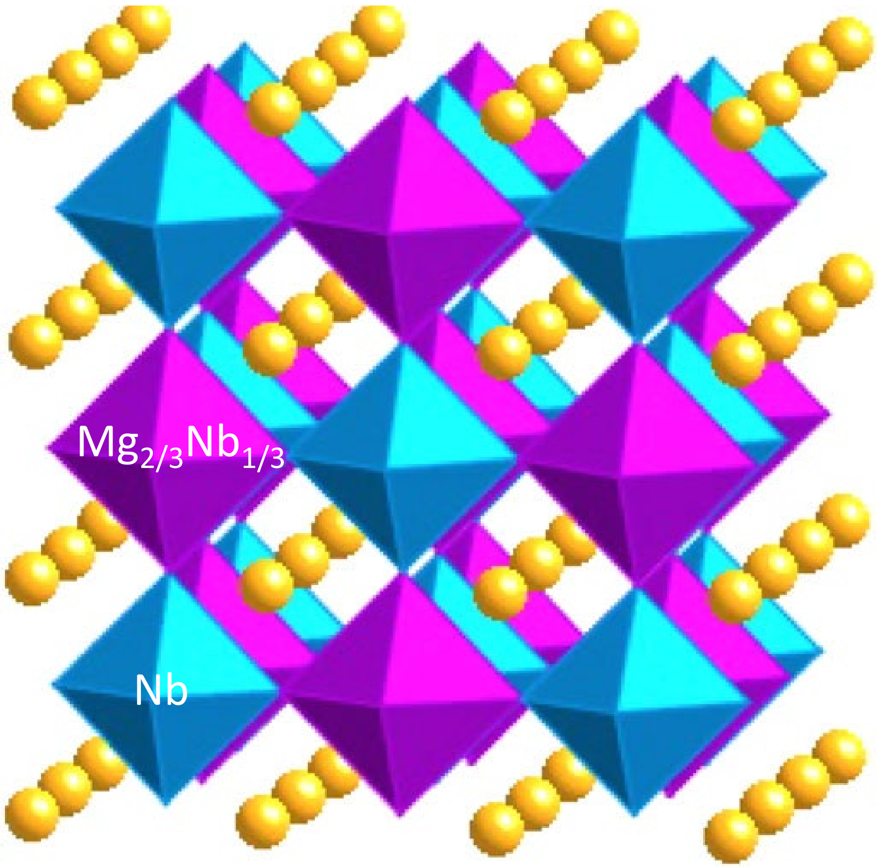
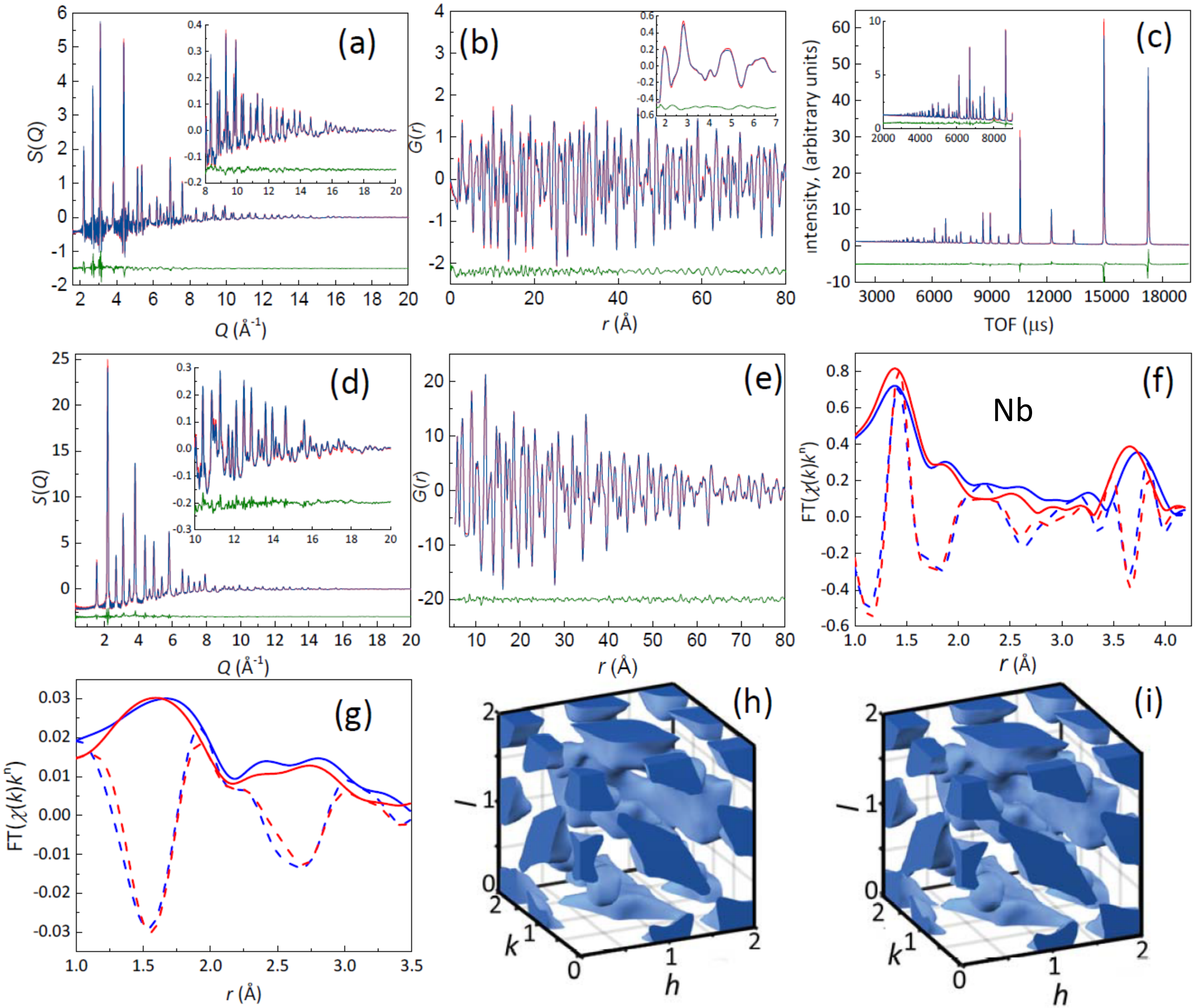
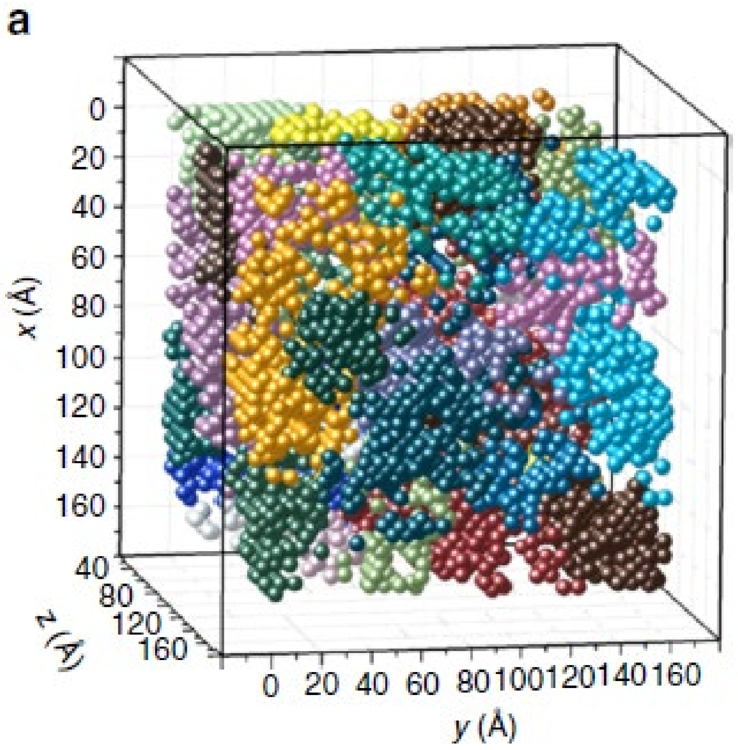
$PbMg_{1/3}Nb_{2/3}O_3$



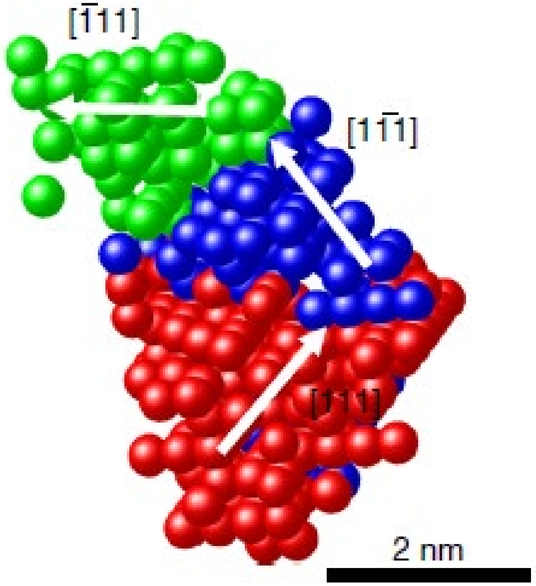

313600 atoms
160 Å x160 Å x160Å



(a)
S(Q)
Q (Å⁻¹)
(b)
G(r)
r (Å)
(c)
intensity, (arbitrary units)
TOF (μs)
(d)
S(Q)
Q (Å⁻¹)
(e)
G(r)
r (Å)
(f)
Nb
FT(χ(k)kⁿ)
r (Å)
(g)
FT(χ(k)kⁿ)
r (Å)
(h)
l
k
h
(i)
l
k
h


a
x (Å)
0
20
40
60
80
100
120
140
160
z (Å)
40
80
120
160
y (Å)
0 20 40 60 80 100 120 140 160

α PNR


$[\bar{1}11]$
$[1\bar{1}1]$
[111]
2 nm

<111> PNR

R. Vedrinskii
A. Mirmilstein
A. Novakovich
L. Bugaev
A. Shuvaev
B. Khelmer (Chudnovsky)
A. Vazina

I. Levin
M. Eremenko
Y. Zhang
M. Tucker

# Thank you for attention