The Study of Incommensurate Modulation in High Tc Superconductors

1. Introduction

** What is a modulated structure?*
** Results from previous studies*

2. Electron Diffraction Analysis using Direct Method

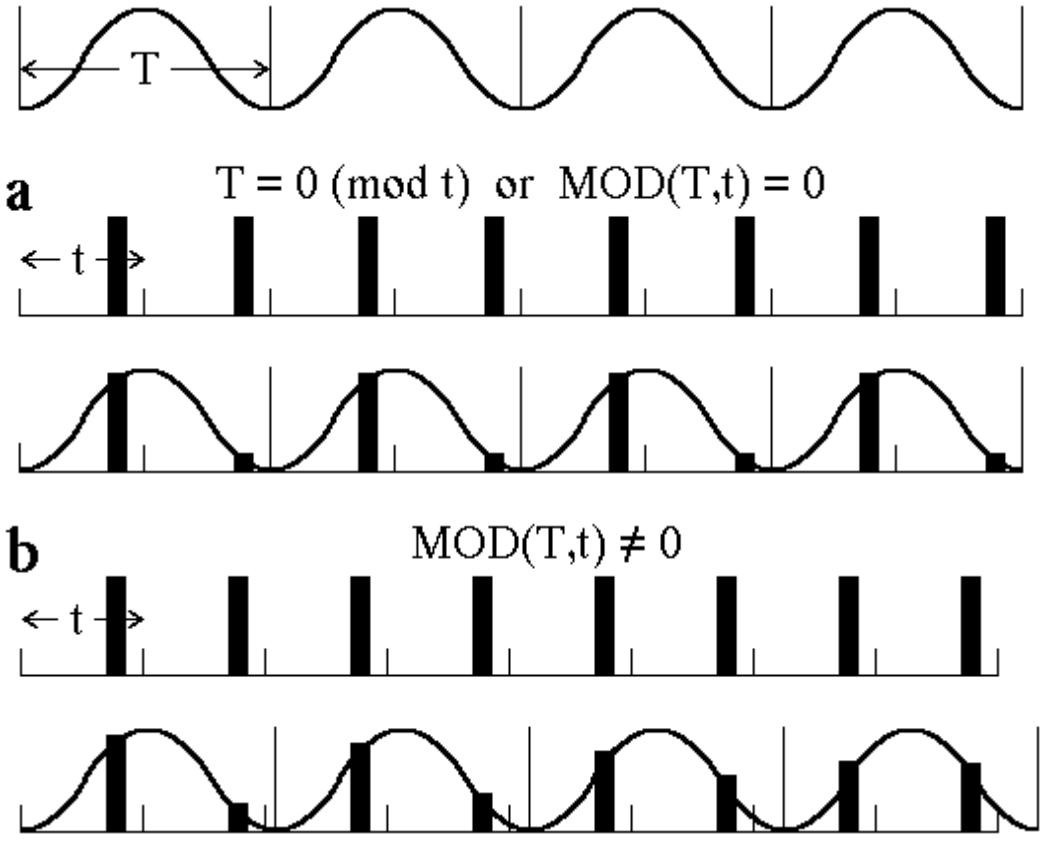
** Why using electron diffraction?*
** Why using direct method?*
** Direct methods for incommensurate modulated structures*

3. Experiment and Results

** Two different modes of modulation in Bi-2223 phase*

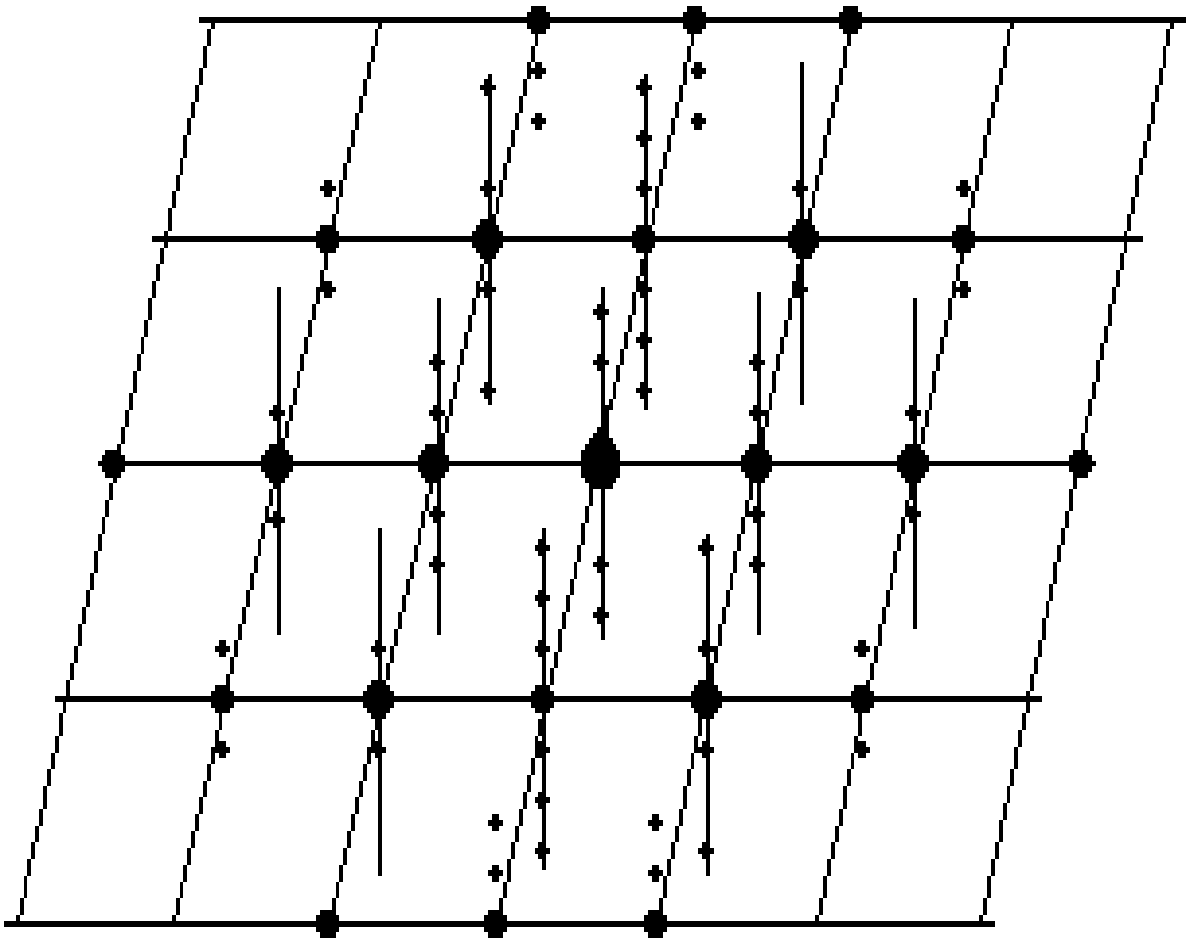
Occupational modulation of a one-dimensional structure

(a) commensurate modulation
(b) incommensurate modulation

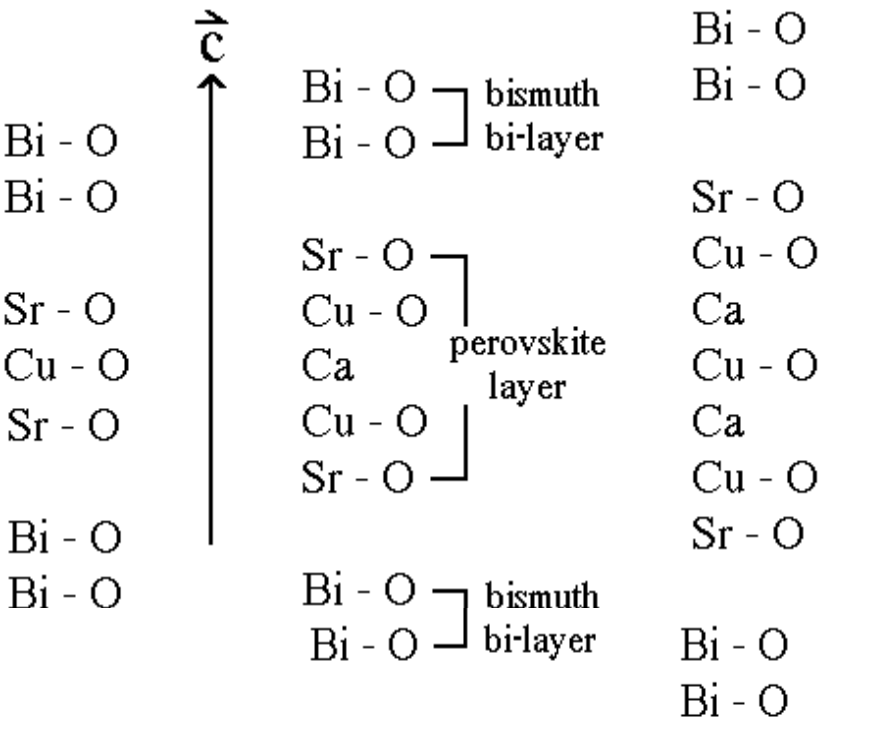


Schematic diffraction photograph
of an incommensurate modulated structure

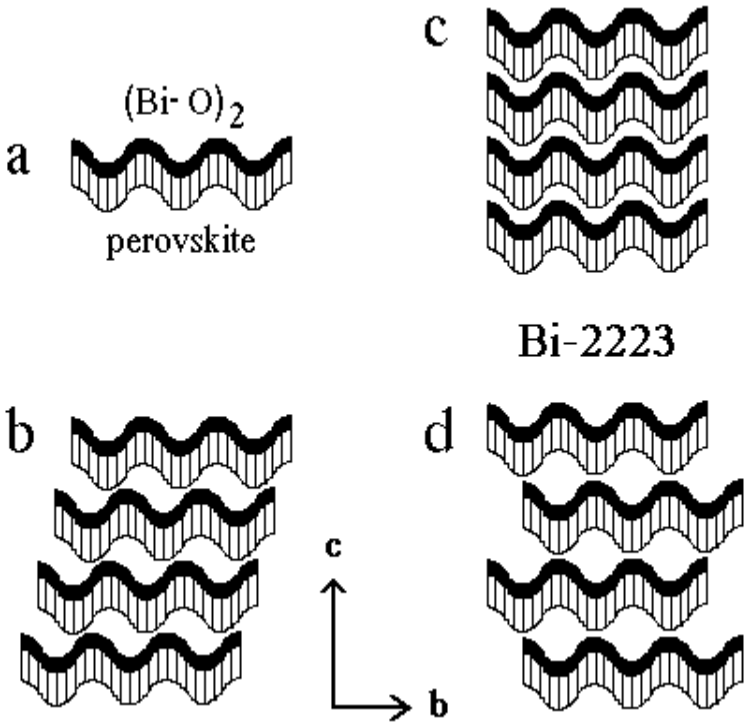
The vertical line segments indicate the projection of lattice lines parallel to the fouth dimension



$Bi_2 Sr_2 Ca_{n-1} Cu_n O_{2n+4}$



Different modes of modulation in the Bi-based superconductors by high resolution electron microscopy

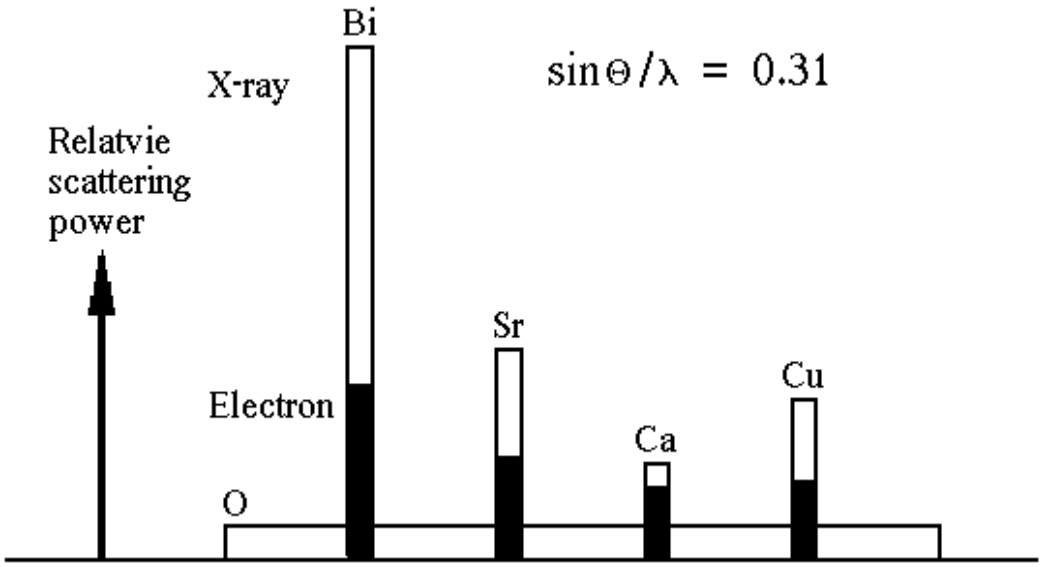


Bi-based Superconductors

$Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$

n = 1	n = 2	n = 3
$Bi_2Sr_2CuO_6$	$Bi_2Sr_2CaCu_2O_8$	$Bi_2Sr_2Ca_2Cu_3O_{10}$
Tc = 20K	Tc ~ 80K	Tc ~ 110K
[1] Y. Gao *et al.* *Physica C* 160, 431 (1989) (X-ray, single crystal)	**[1] Y. Gao *et al. Science* 241, 954 (1988) (X-ray, single crystal)**	**Y.D. Mo *et al.* *Supercond. Sci. Technol.* 5, 69 (1992) (Electron, micro-crystal, direct method)**
[2] A. Yamamoto *et al.* *Physica C* 201, 137 (1992) (Neutron and X-ray, Rietveld method)	**[2] A. Yamamoto *et al. Phys. Rev. B* 42, 4228 (1990) (Rietveld method)**	
	[3] P. Lee *et al. Acta Cryst.* A47, 57 (1991) (Synchrotron radiation. epitactic film)	
	[4] X.B. Kan *et al.* *Acta Cryst.* B (1993) (X-ray, single crystal)	
	[5] Y.Gao *et al. Acta Cryst.* A49, 141 (1993)	

The relative scattering power of the elements Bi, Sr, Ca, Cu and O for X-rays and electrons



The Phase Problem

$$\mathrm{F}(\mathbf{H}) = \sum_{j=1}^{N} f_j \, e^{i\, 2\pi \mathbf{H}\cdot\mathbf{r}_j}$$

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{H}} \mathrm{F}(\mathbf{H}) \, e^{-i\, 2\pi \mathbf{H}\cdot\mathbf{r}}$$

Sayre equation

$$\mathrm{F}(\mathbf{H}) = \frac{\theta}{V} \sum_{\mathbf{H'}} \mathrm{F}(\mathbf{H'}) \, \mathrm{F}(\mathbf{H} - \mathbf{H'})$$

Tangent formula

$$\tan \phi_{\mathbf{H}} \approx \frac{\left\langle E_{\mathbf{H'}} E_{\mathbf{H}-\mathbf{H'}} \sin(\phi_{\mathbf{H'}} + \phi_{\mathbf{H}-\mathbf{H'}}) \right\rangle_{\mathbf{H'}}}{\left\langle E_{\mathbf{H'}} E_{\mathbf{H}-\mathbf{H'}} \cos(\phi_{\mathbf{H'}} + \phi_{\mathbf{H}-\mathbf{H'}}) \right\rangle_{\mathbf{H'}}}$$

Direct methods for incommensurate modulated structures

$$F(\hat{\mathbf{H}}) = \frac{\theta}{V}\sum_{\mathbf{H}'} F(\hat{\mathbf{H}}')\,F(\hat{\mathbf{H}}-\hat{\mathbf{H}}')$$

$$= \frac{\theta}{V}\sum_{\mathbf{H}'} F_m(\hat{\mathbf{H}}')\,F_m(\hat{\mathbf{H}}-\hat{\mathbf{H}}')$$

$$2\sum_{\mathbf{H}'} F_m(\hat{\mathbf{H}}')\,F_s(\hat{\mathbf{H}}-\hat{\mathbf{H}}') +$$

$$\sum_{\mathbf{H}'} F_s(\hat{\mathbf{H}}')\,F_s(\hat{\mathbf{H}}-\hat{\mathbf{H}}')$$

$$F_m(\hat{\mathbf{H}}) \approx \frac{\theta}{V}\sum_{\mathbf{H}'} F_m(\hat{\mathbf{H}}')\,F_m(\hat{\mathbf{H}}-\hat{\mathbf{H}}')$$

$$F_s(\hat{\mathbf{H}}) \approx 2\frac{\theta}{V}\sum_{\mathbf{H}'} F_m(\hat{\mathbf{H}}')\,F_s(\hat{\mathbf{H}}-\hat{\mathbf{H}}')$$

Hao, Q., Liu, Y.W. and Fan, H.F.,
***Acta Cryst.*, A43, 820-824 (1987)**

Sample:

Bi-2223 phase with nominal composition of

$$Bi_{1.6}Pb_{0.4}Sr_2Ca_2Cu_3O_y$$

Electron diffraction:

Diffraction patterns taken with a
Hitachi H-9000 electron microscope

Space Group: *P:Bbmb:1-11*

Unit cell:

a=5.49, b=5.41, c=37.1A

$\alpha=\beta=\chi=90^o$

$q=0.117b^*$

Intensity measurement:

by a Perkin Elmer PDS microdensitometer

using a 20x20 μm^2 aperture

42 main reflections and 70 satellites were obtained