

# Diffuse Scattering

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## 1. Introduction

Most of the materials include some disorder or/and fluctuation in their crystalline structures, which more or less affects the physical and chemical properties. The structural disorders are ideally investigated through the X-ray diffuse scattering measurements. Diffuse scatterings are, in general, widely broaden in reciprocal space, but some of them are concentrated as relatively sharp maxima. The former is generally very weak and the latter must be measured with a considerably high resolution. Therefore, these extreme cases of requirements must be considered in designing the beamline system for the diffuse scattering experiments.

We here propose a new word of 'excited lattice'. We first consider a perfect crystal as a ground state. The disorder or fluctuation in the lattice can be regarded as a kind of excitation due to some 'external force'. The external force may be caused by a variety of environmental and internal conditions of the crystal, e.g. temperature, pressure, magnetic field, electric field, surrounding gas, crystal growth process, atomic composition, doping impurities, irradiation and so on. Modifications of the lattice due to these external forces will appear in various kinds of manners, such as (order-disorder, magnetic, etc.) phase transitions, cascades, dislocations, short-range order, precipitations, recrystallization, diffusion, etc. We will call the fluctuating and/or disordered lattice as 'an excited lattice'. We will be able to systematically understand all the crystalline materials causing the X-ray diffuse scatterings as the excited lattices.

The environmental conditions (causing the

external forces defined above) on the sample in the experiments could control a mode of the lattice excitation. That is, in-situ observations of the fluctuations with changing conditions give us a deeper insight into the kinetics.

The higher energy and higher flux photon beams generated in the SPring-8 are suitable for probing the excited lattice states in bulky samples surrounded with heavy or massive instruments creating the environmental conditions. In particular, an anomalous dispersion term of atomic scattering factor is effective to enhance weak diffuse scatterings, which is coming from the tunability of SR beam. We investigate the relationship between the physical properties and structural fluctuations in materials.

## 2. Research projects

Our research group covers the following lattice excitations :

- 1) Disorders in practical alloys, advanced and/or functional materials ; Precipitations, Ion implantations, Point defects and defect clusters, impurity precipitations and fluctuations related to order-disorder phase transitions.
- 2) Structural fluctuations for intercalation compounds, super-lattice and multi-layered materials .

## 3. Experimental setup

We need a conventional and large four-circle diffractometer to install the attachments for the present diffuse scattering experiments. Following detectors will be used : a) scintillation detector, b) solid state detectors and c) imaging plates. These detectors will be effective for measuring the diffuse intensities with higher energy resolution or low background.

## 4. Experiment

We are now planning to perform the diffuse intensity measurements from disordered ternary alloys (Pe-Ni-Cr and Cu-Ni-Pt) with X-rays of

different energies by taking an advantage of anomalous dispersion effect as the first experiment at the Spring- 8 because there are few reports for the study by X-ray and neutron diffraction experiments [1, 2]. Diffuse intensity will be collected at least within the first Brillouin zone in a reciprocal space . After correcting several factors to the observed intensity, we can get data in an absolute unit. Partial short-range order parameters will be taken by the Fourier transform of the data. BY computer simulation, we construct a possible local structure for the disordered ternary alloys. We also discuss the phase stability from a thermodynamical point of view with the use of the parameters.

#### **4. Remark**

In a near future, multi-component materials of great commercial significance will be proposed from a continuous of the diffuse intensity measurements and analyses for the alloys .

#### **References**

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- [2] S. Hashioto, H. Iwasaki, K Ohshima J. Harada, M. Sakata and H. Terauchi : J. Phys. Soc. Jpn. 54, 3796 (1985).