X線異常散乱法による機能性カルコゲンガラスの局所構造の解明

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散乱実験によるガラスなどの非晶質合金の原子配列の研究で最も重要なことは、その成分元素の原子構造を明確に区別することである。N元系ガラスの場合には $N(N+1)/2$ 個の散乱断面積が異なる手法を準備する必要があり、例えばX線、中性子回折を行っても、2成分ガラスにおいてもその情報は十分ではない。

X線異常散乱法は、成分元素のX線吸収端付近で起こる原子形状因子の異常を用いて、元素選択的な散乱実験を可能にする。しかしながら、弾性散乱成分をコンプトン散乱や蛍光X線から正確に選り分ける必要がある。われわれは、2台のシリコン・ドリフト半導体検出器を、散乱測定および後方散乱位置に配置し、弾性散乱成分を効率よく正確に取り出すことを試み、スキャン終了後 30 分以内に、原子形状因子の異常効果による散乱強度のコントラスト（差構造因子）を得ることに成功した[1]。発表では、赤外線光ファイバー材料Ga-Ge-Seについての測定結果を実験例として報告する。

[1] J. R. Stellhorn, S. Hosokawa, and E. Magome, AIP Conf. Proc.,投稿中.

A partial structural study of functional chalcogenide glasses by anomalous x-ray scattering

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Abstract

For structural investigations on non-crystalline materials such as glasses and liquids, the most important task is to clarify partial atomic structures. For N-component alloys, totally N(N+1)/2 of diffraction experiments is necessary with different scattering cross-sections. For example, x-ray and neutron diffraction experiments are not enough to partial structures of a binary alloy.

Anomalous x-ray scattering (AXS) utilizes anomalous behavior of an atomic form factor close to an absorption edge of a constituent element, and enables an element-selective diffraction experiments [1]. This method is, in particular, very effective for alloys of Ga, Ge, As, and Se, which have scattering cross-sections for x-rays and neutrons very similar to each other.

To obtain differential structure factor close to an absorption edge, $\Delta_k S(Q)$, however, the elastic scattering signal should be carefully discriminated from the fluorescent and Compton scattering contributions. For this, two silicon-drift detectors (SDD) were used for measuring the scattering signal at scattering angle 2θ and for monitoring fluorescent x-rays at the backscattering geometry [2]. Using such a detecting system, we were able to obtain $\Delta_k S(Q)$ within 30 min after finishing the data collections.

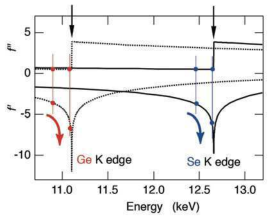
[1] Y. Waseda, Anomalous X-Ray Scattering for Materials Characterization (Berlin-Heidelberg, Springer, 2002).

[2] J. R. Stellhorn, S. Hosokawa, and E. Magome, AIP Conf. Proc., submitted.

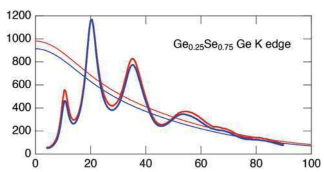
Principle of AXS

$f(Q,E) = f_0(Q) + f'(E) + if''(E)$

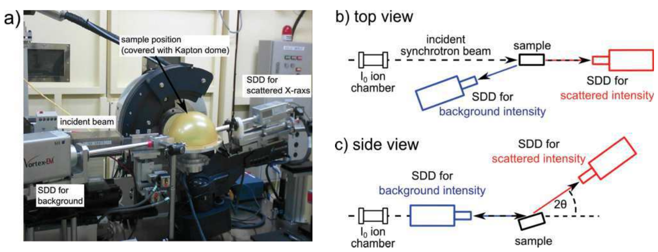
Usual terms   Anomalous terms



Normalized scattering data

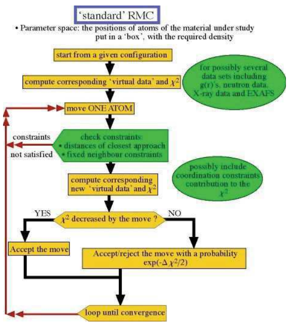


AXS experiment at BL15/Saga-LS



Reverse Monte Carlo (RMC) modeling to obtain $S_{ij}(Q)$

Algorithm



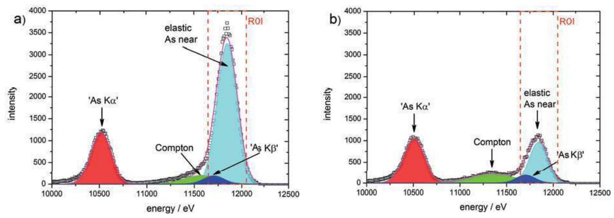
Program
RMC++ package

Number of atoms
Totally 5000 atoms

Initial configuration
Random hard-sphere

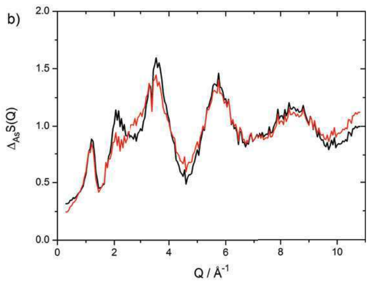
Constraints
Cut off length ~0.22 nm

Experimental data



Scanning detector   Backscattering detector

$\Delta_k S(Q)$

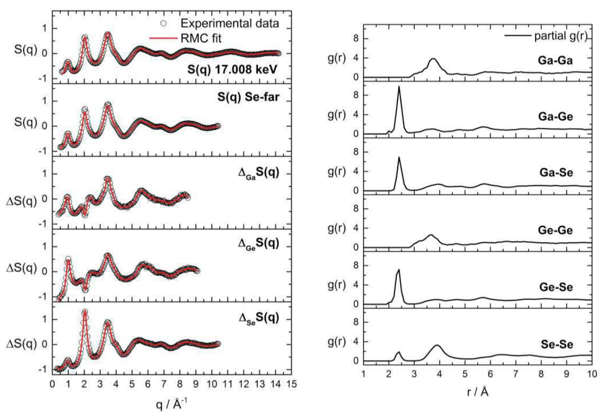


roughly corrected

precisely corrected

As edge of $As_{25}Se_{75}$ glass

Experimental data of Ga-Ge-Se glass measured at ESRF



Detecting system at ESRF