Characterization of Materials for Novel Devices by XAFS and Ab-initio Calculation

XAFS Application to $Si_{0.95}Ge_{0.05}$ Thin Film

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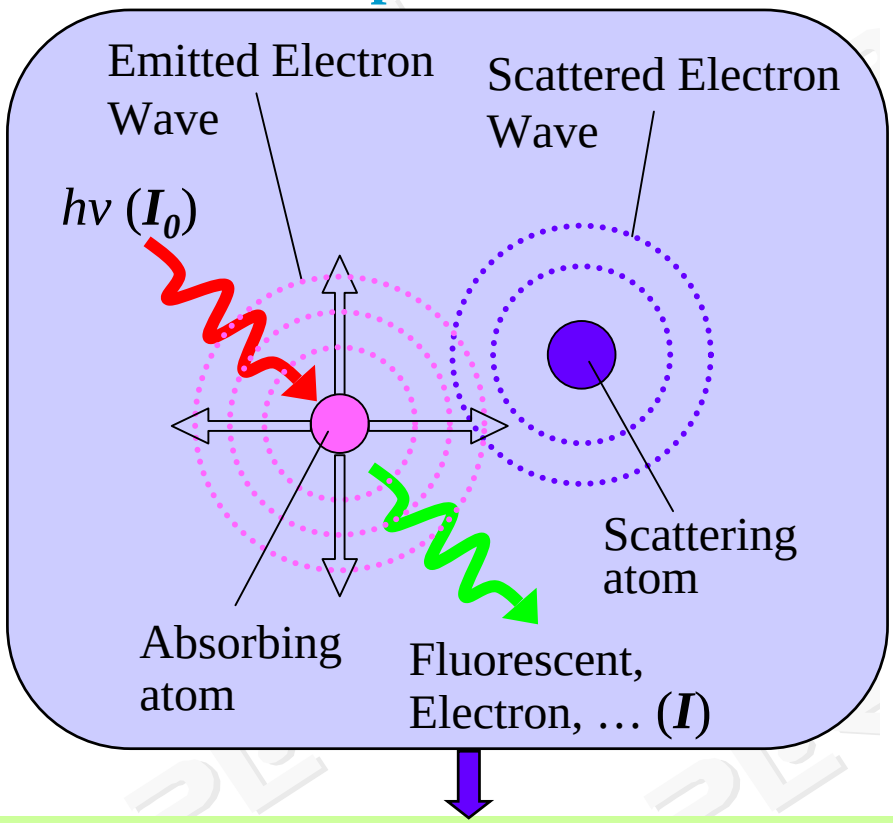
Outline

- Principle XAFS and Theoretical Background
- XAFS Application to $Si_{0.95}Ge_{0.05}$ Film
- Summary

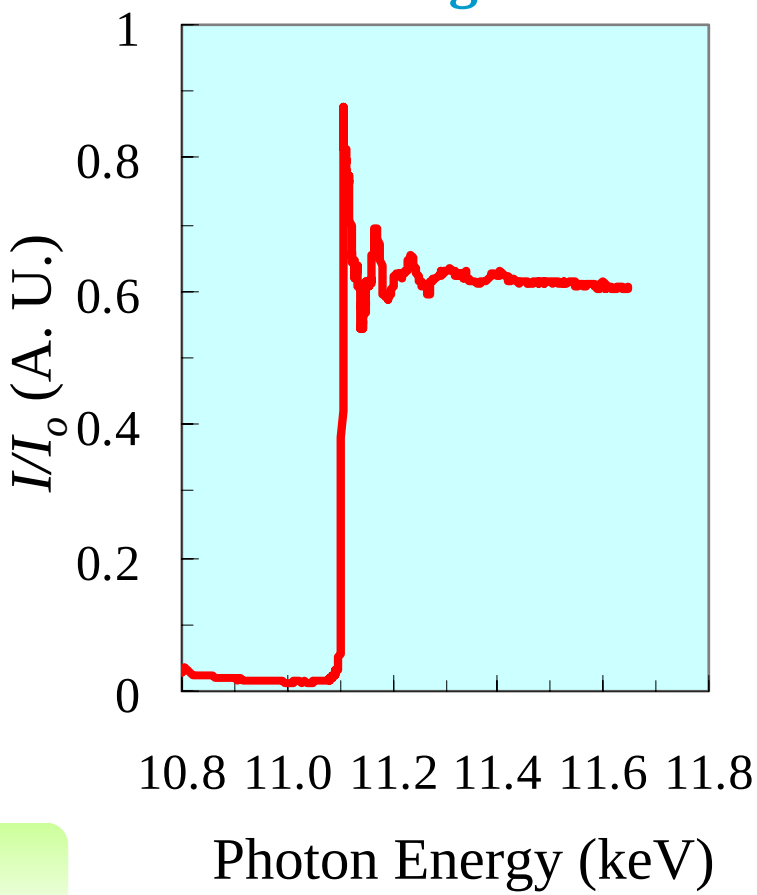
Principle XAFS and Theoretical Background

Principle of XAFS



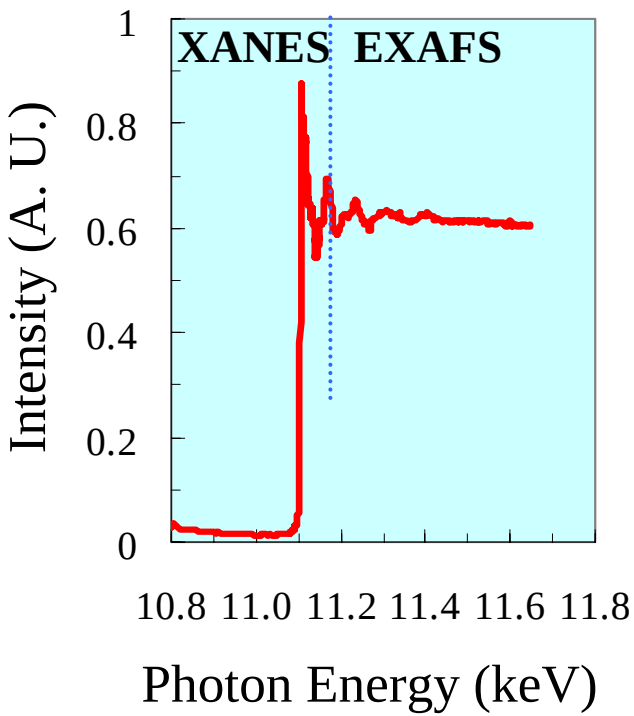
Interference of electron waves perturbs absorption intensity (I/I_0) and yields XAFS.

Ge *K*-edge XAFS



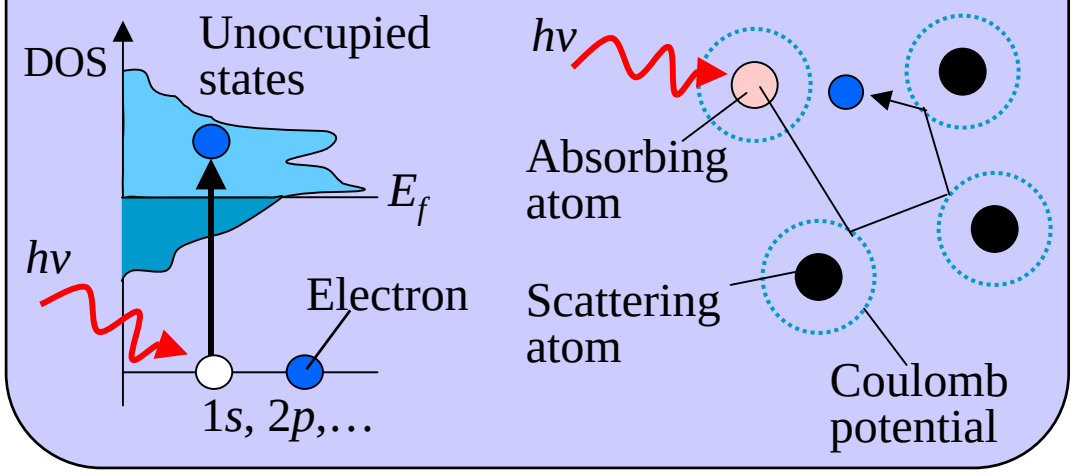
Principle XAFS and Theoretical Background

EXAFS and XANES



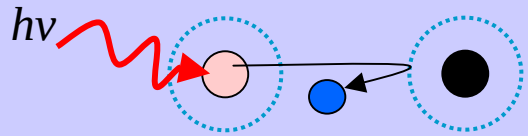
XANES

Electronic transition/Multiple scattering



EXAFS

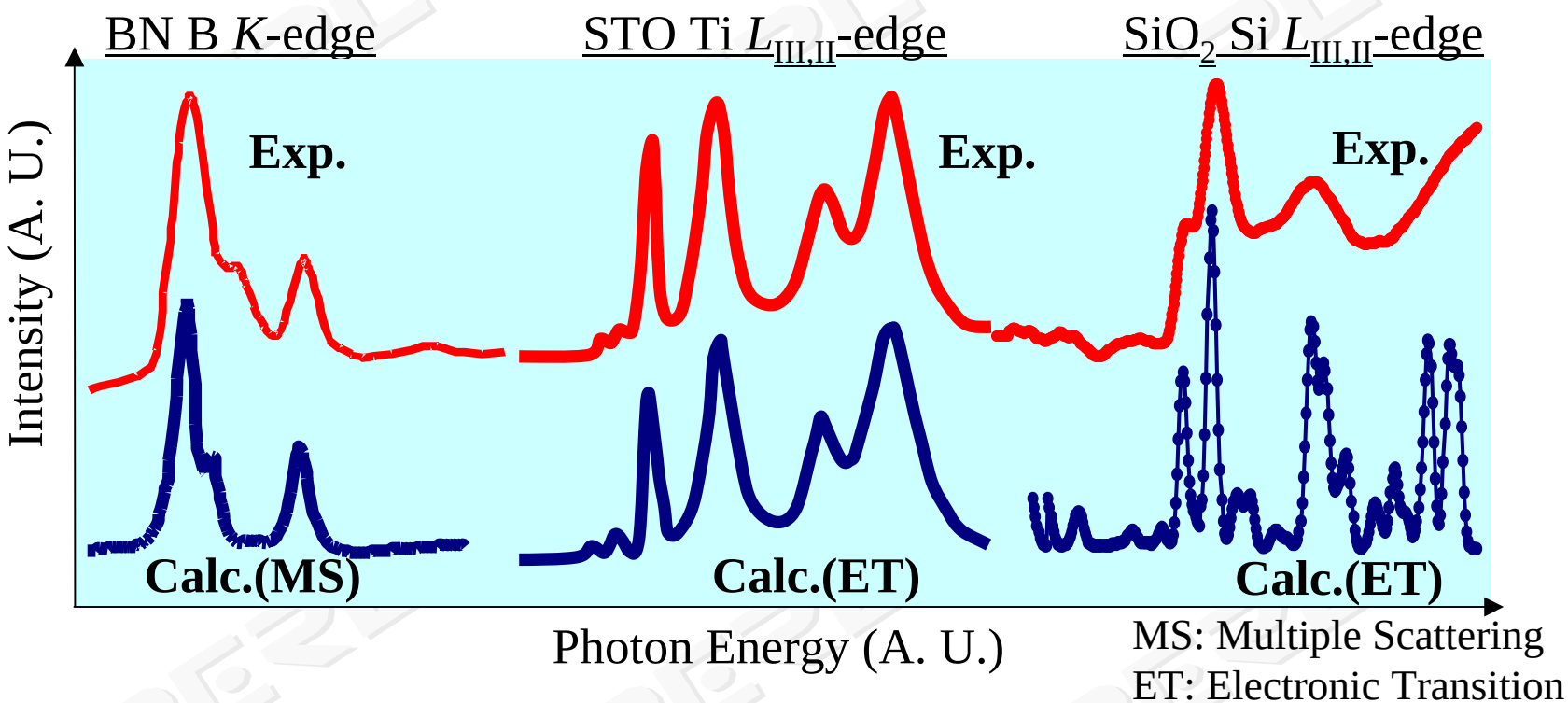
Single scattering



We developed programs for XANES calculations and applied to analysis.

Principle XAFS and Theoretical Background

Experimental and calculated XANES spectra

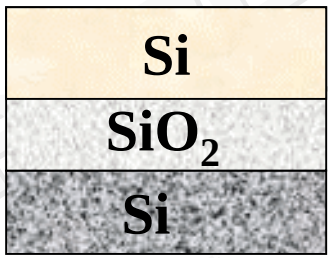


Calc. can reproduce experimental data fairy well.

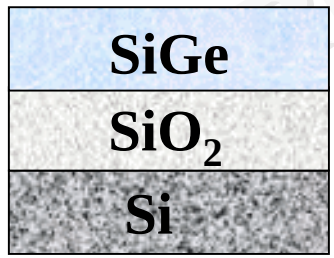
→It is possible to obtain electronic and structural information from XANES.

XAFS Application to $Si_{0.95}Ge_{0.05}$ Film:Introduction

Poly-Si gate



Poly-SiGe gate



Problem of poly-Si gate

1. High temperature deposition
2. Carrier depletion

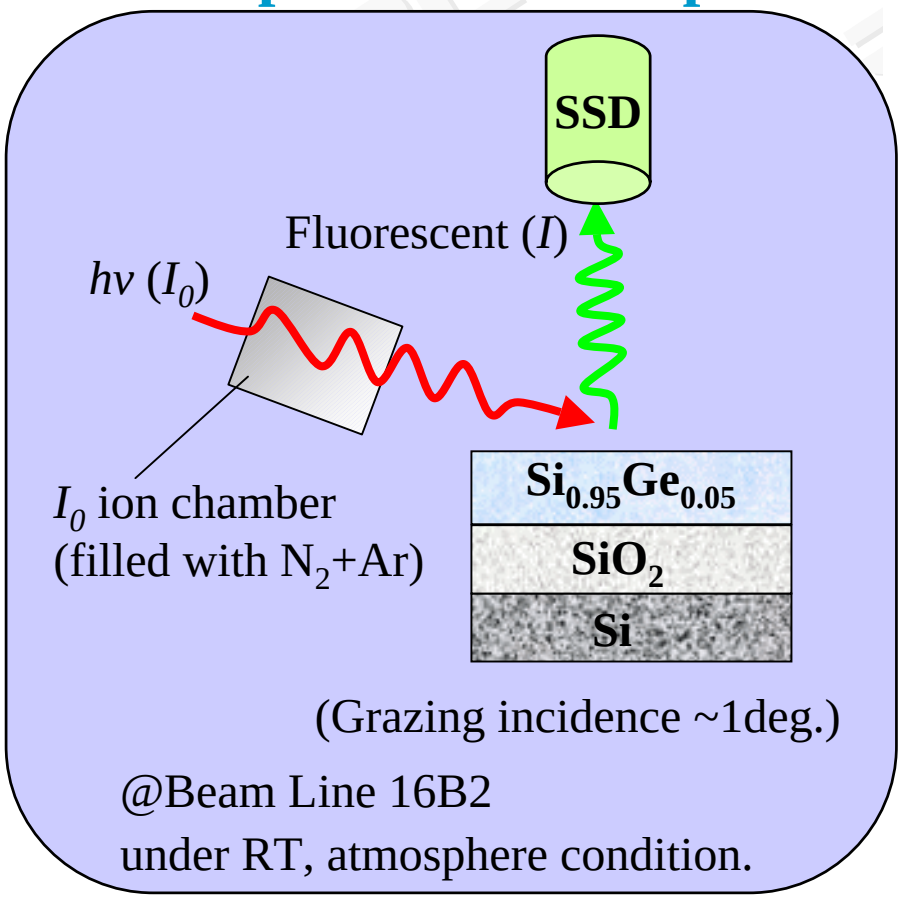
Features of poly-SiGe gate

1. Low temperature deposition
2. Suppression of carrier depletion

In order to understand properties of SiGe,
we applied XAFS to $Si_{0.95}Ge_{0.05}$ to obtain the structural information.

XAFS Application to $Si_{0.95}Ge_{0.05}$ Film:Experimentals

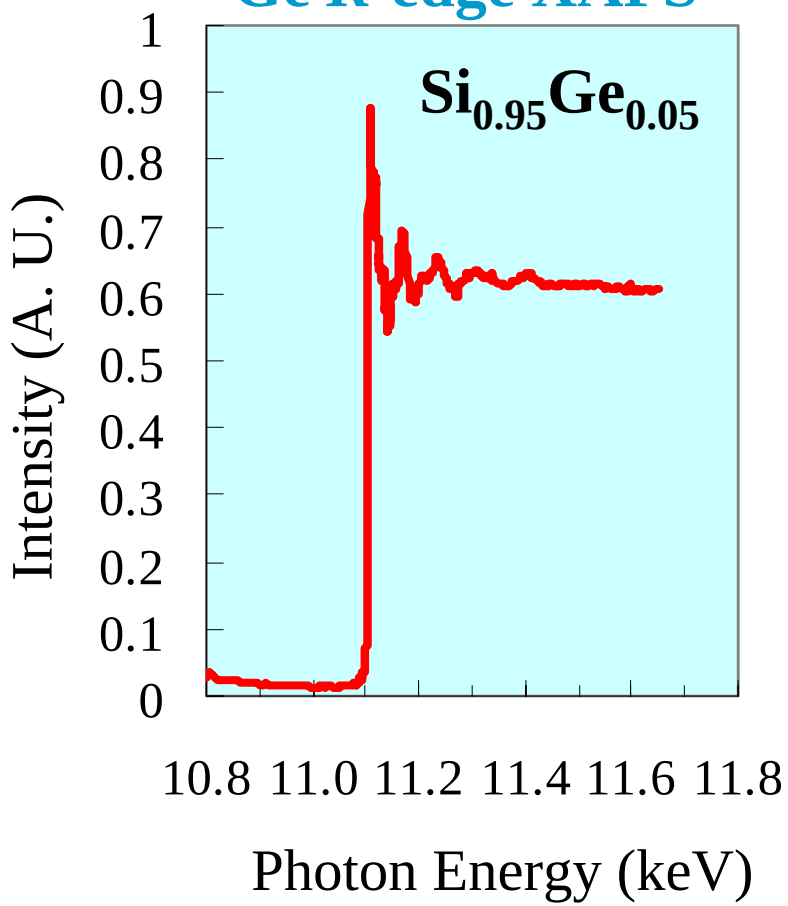
Experimental setup



(Grazing incidence ~1deg.)

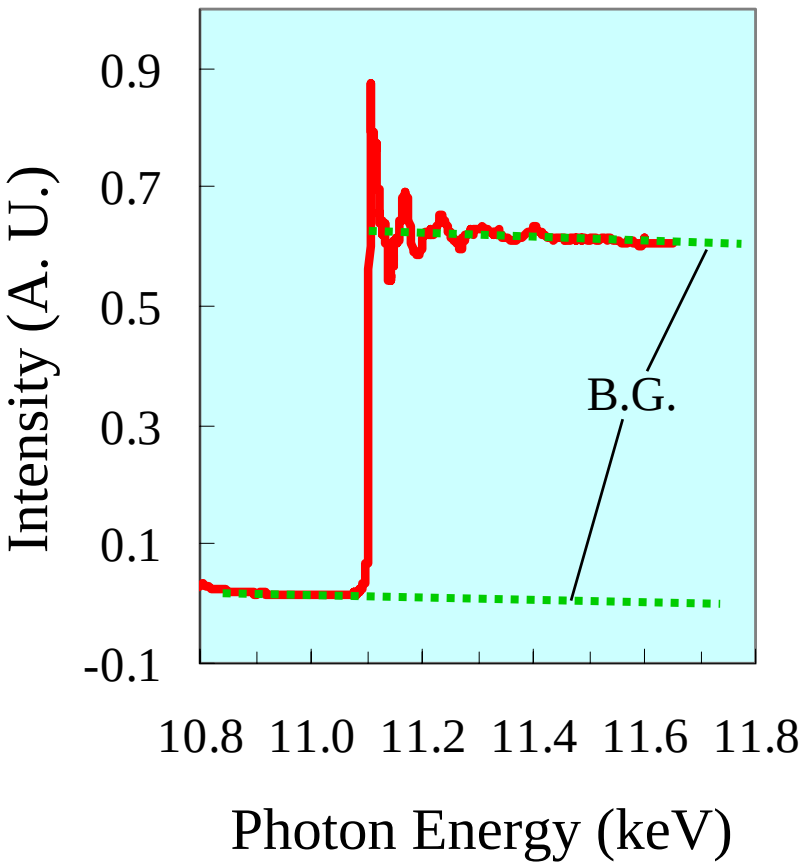
@Beam Line 16B2
under RT, atmosphere condition.

Ge *K*-edge XAFS

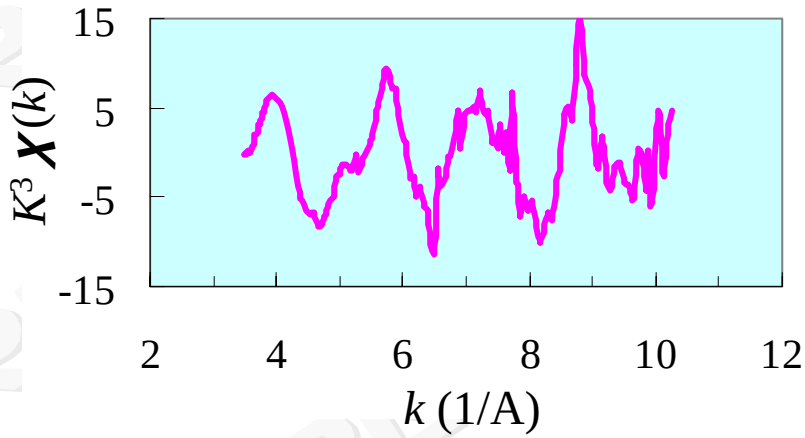


XAFS Application to $Si_{0.95}Ge_{0.05}$ Film:Experimentals

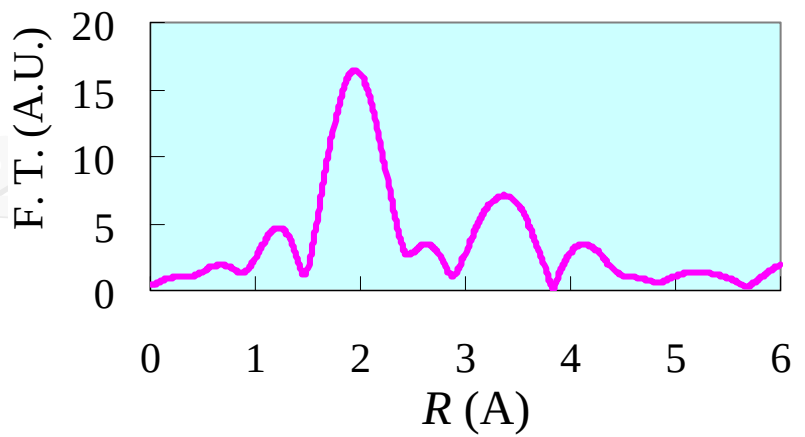
Raw data and background



Extracted EXAFS function

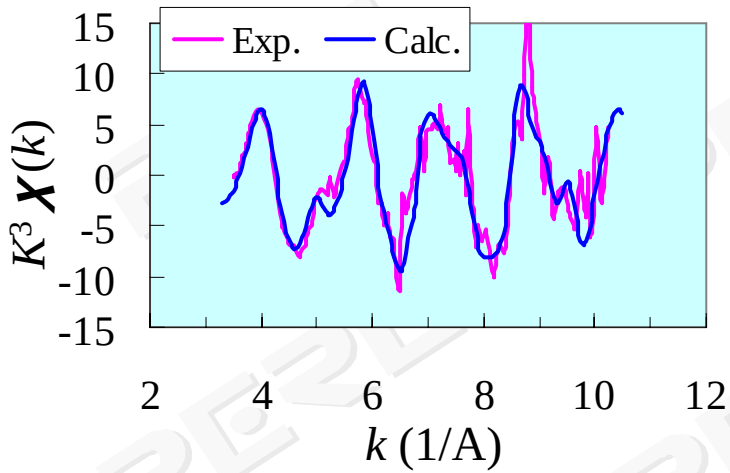


Fouriertransformed EXAFS function

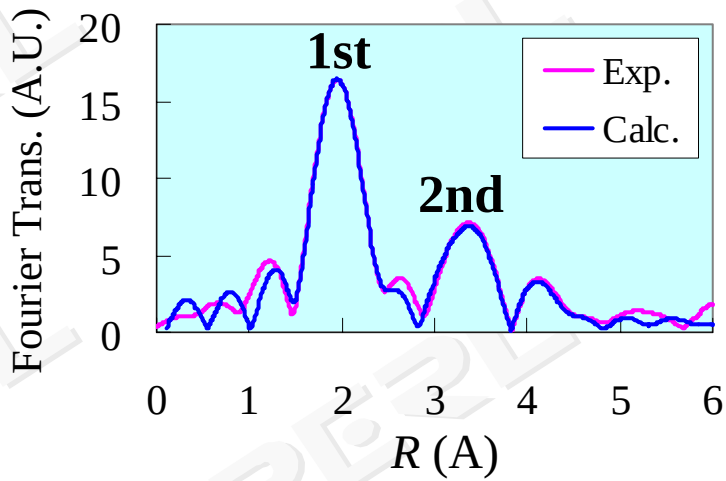


XAFS Application to $Si_{0.95}Ge_{0.05}$ Film:Results

Extracted EXAFS function



Fourier transformed EXAFS function



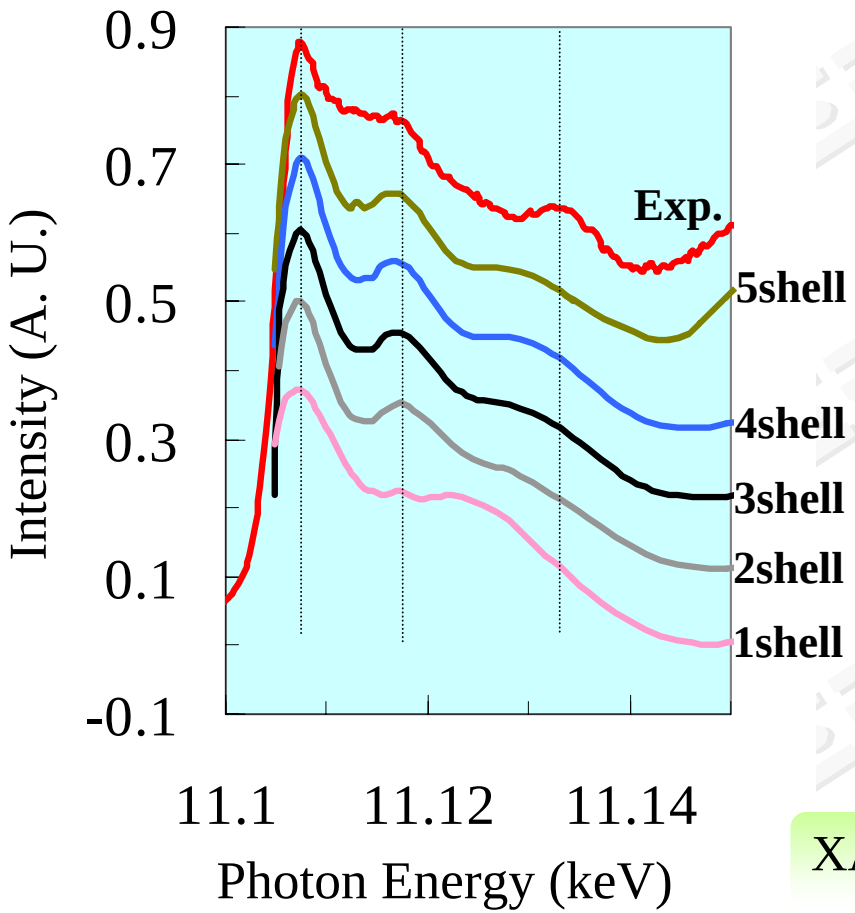
Curve fitting Results

	Shell	S_0^2N	R (A)	ΔE (eV)	C_2 ($\times 10^2$A^2)	R-fac (%)
1st Peak	Ge-Si	3.40	2.363	4.60	0.22	0.5%
	Ge-Ge	0.31	2.418	-0.42	~0	
2nd Peak	Ge-Si	7.52 (0.25)	3.809 (0.003)	-0.21 (0.30)	0.68 (0.25)	2.1%

S_0^2N(Ge-Si)$\gg S_0^2N$(Ge-Ge)→Ge-Ge bonds can be neglected.

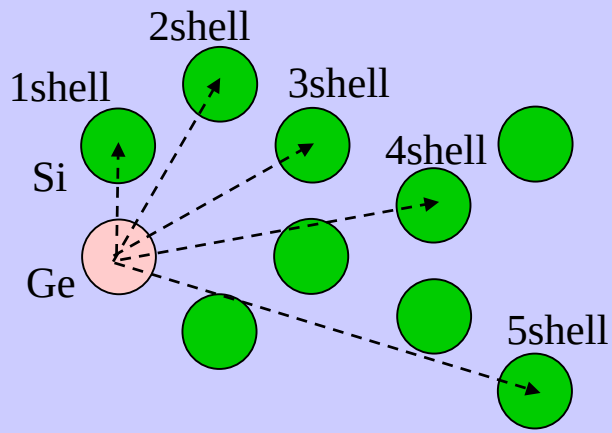
XAFS Application to $Si_{0.95}Ge_{0.05}$ Film:Results

Exp. and Calc. XANES spectra



Calculation Model

5Shell・・・Ge in Si_{46} matrix
4Shell・・・Ge in Si_{34} matrix
3Shell・・・Ge in Si_{28} matrix
2Shell・・・Ge in Si_{16} matrix
1Shell・・・Ge in Si_4 matrix



XANES Calculation needs more than 5shell.

XAFS Application to $Si_{0.95}Ge_{0.05}$ Film:Results

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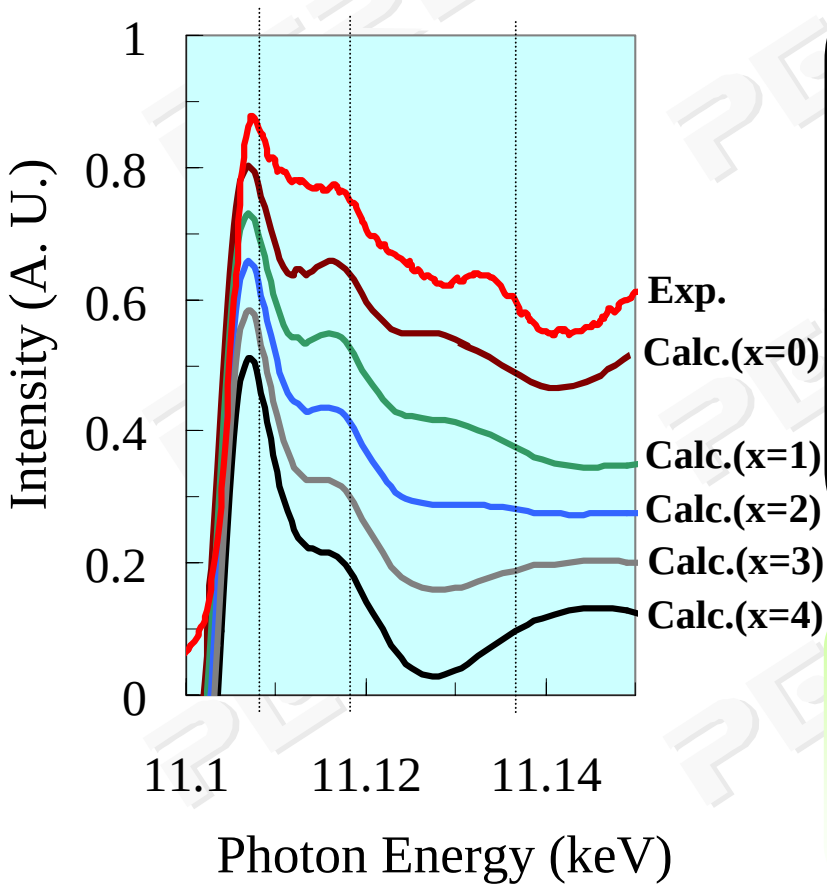
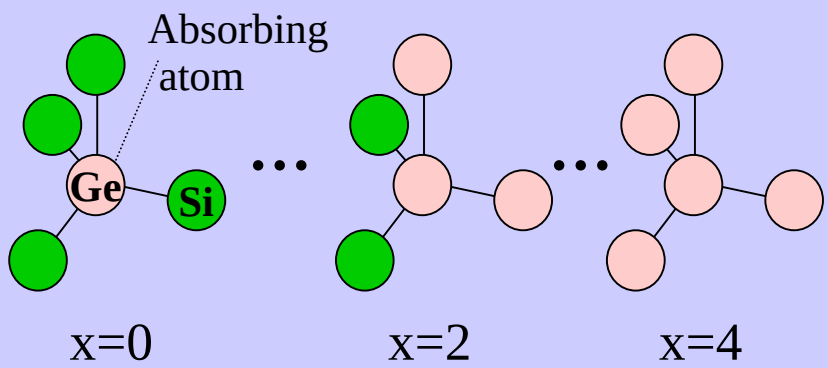


Calculation Model

$Si_{5-x}Ge_x$ cluster in Si_{42} matrix (5shell)



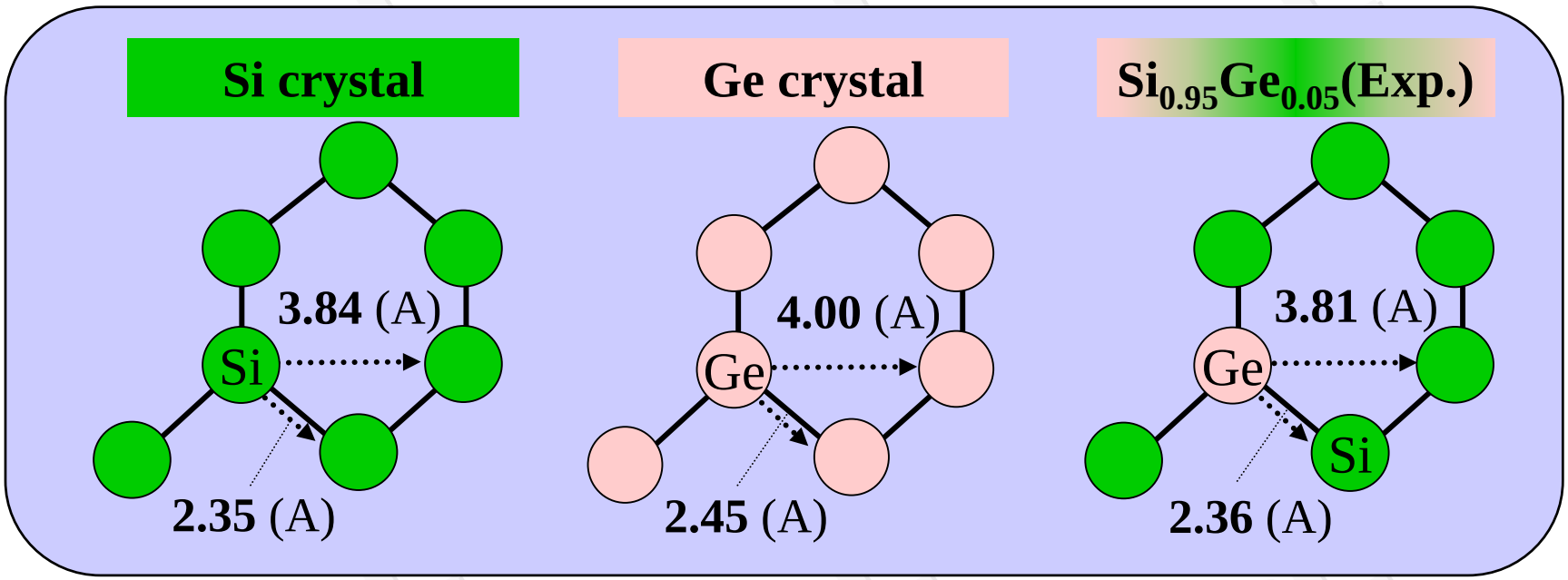
x:Number of Ge around absorbing atom

Calc.(x=1) can reproduce Exp. well.

➡ XANES confirms EXAFS result,
S_0^2N(Ge-Si)≫S_0^2N(Ge-Ge).

XAFS Application to $Si_{0.95}Ge_{0.05}$ Film:Atomic Structure

Local atomic structure of Si, Ge, $Si_{0.95}Ge_{0.05}$



$Si_{0.95}Ge_{0.05}$ structure is almost same with Si.

This largely strained structure may has the effect on electrical properties.

Summary

We applied XAFS and Ab-initio calculations to $Si_{0.95}Ge_{0.05}$ film and following conclusion was obtained.

Local structure of $Si_{0.95}Ge_{0.05}$ is almost coincidence with crystalline Si structure and highly strained.