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準結晶とバルク金属ガラスの軟X線発光分光

To understand *the microscopic origin of their structural stabilities and unique properties*

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- 岩住 俊明（阪府大）

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Agenda

複雑合金系の電子構造と原子配列

- **２次元準結晶** 2-D QuasiCrystal
- **バルク金属ガラス** Bulk Metallic Glass

軟X線発光分光 XES＋**光電子分光** PES

＋**第一原理クラスター計算** DV-*Xα*

To understand *the microscopic origin of*

their structural stabilities

and unique properties

まとめ（XES**への期待**）

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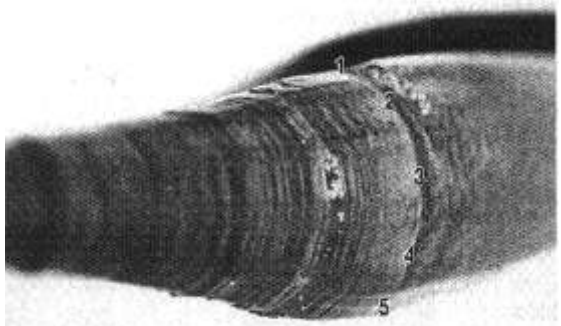
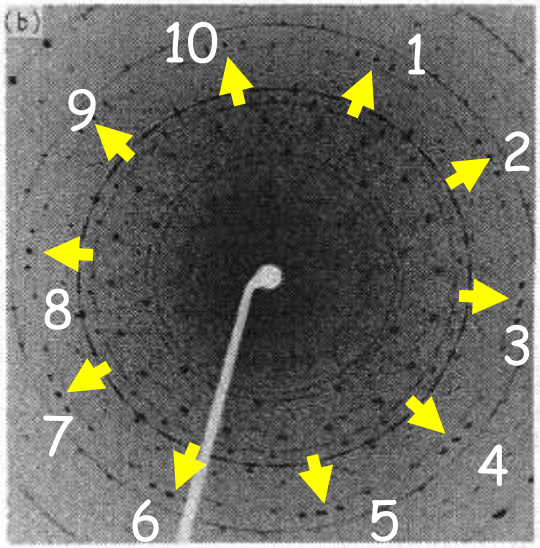
2-D QC Al-Co-Ni

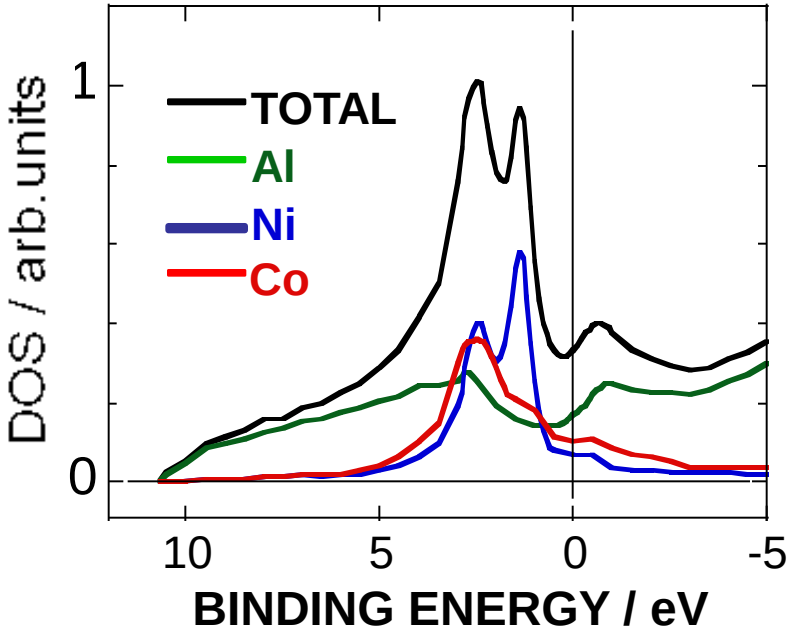


an ingot of $Al_{72}Co_{16}Ni_{12}$



X-ray Laue diffraction pattern taken from the 10-fold axis.

Approximant $Al_{68.60}Co_{14.88}Ni_{16.52}$ [1]



Pseudogap in Al pDOS ?

>>> Hume-Rothery-type stabilizing mechanism

Strong Co-Al interaction ?

>>> Ni central ring

Microscopic origin for unique atomic arrangement ?

[1] M.Krajci *et al.*, Materials Sci. & Eng. **294-296**, 548 (2000).

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Pd-M-P (M = Ni, Cu) BMG

Critical cooling rate

10^6 K/s → 10 K/s

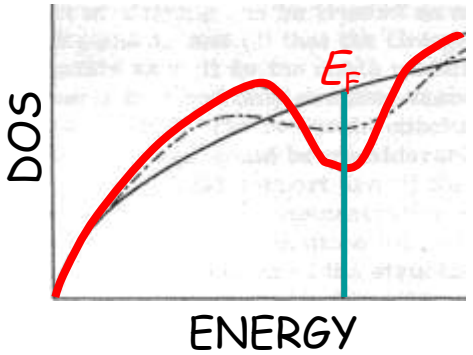
Amorphous Metal

Bulk Metallic Glass

High resistance to crystallization
of thermodynamically metastable BMG

Microscopic origin for large stability ?

- Structure-induced Minimum in Free Electron DOS [1]
  Pseudo-Gap Formation ?
- Role of TM *d* States ?



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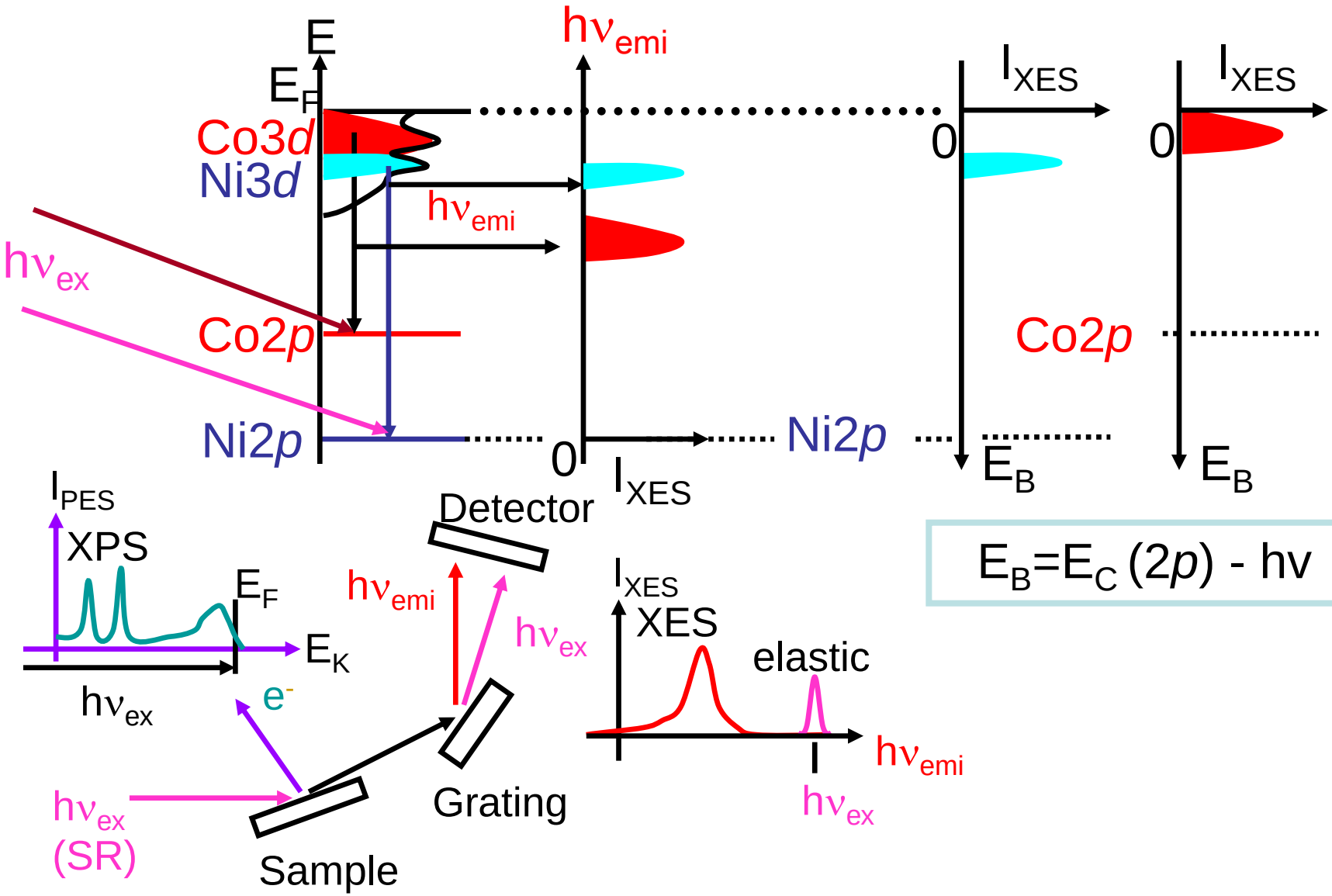
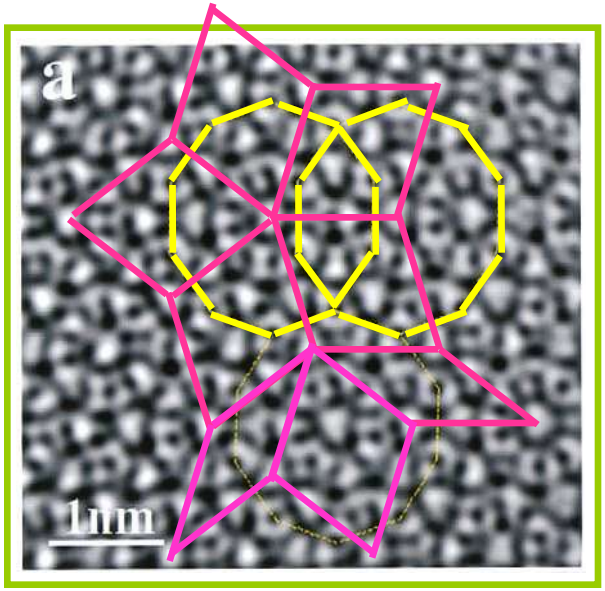
XES measurement



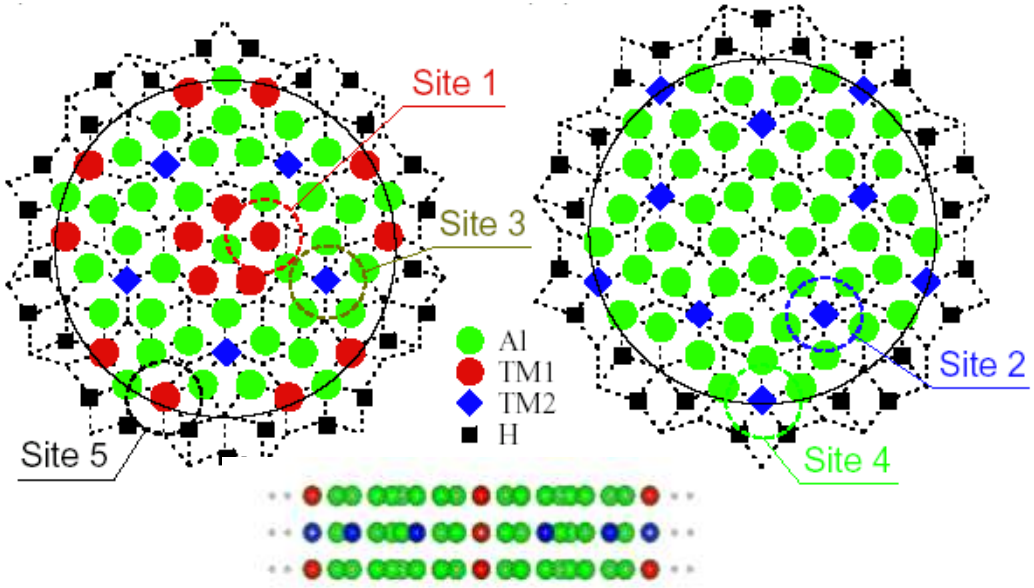
$E_B = E_C\,(2p) - h\nu$

Cluster Calculation

- Discrete Variational $X\alpha$ (DV-$X\alpha$) method [1]
- the available code SCAT [2] tuned up
  for faster calculation with lager cluster



TEM image of Al-Co-Ni [3]



B-A-B cluster > A-layer DOS

+

A-B-A cluster > B-layer DOS

Triple-layer Unit Cluster [4]

[1] H. Adachi *et al.*, J. Phys. Soc. Jpn. **45** (1978) 875-883.
[2] http://www.dvxa.org/
[3] E. Abe *et al.*, Phys.Rev. Lett **84** (2000) 4609.
[4] M. Inukai *et al.*, Z. Kristallogr. *in press*.

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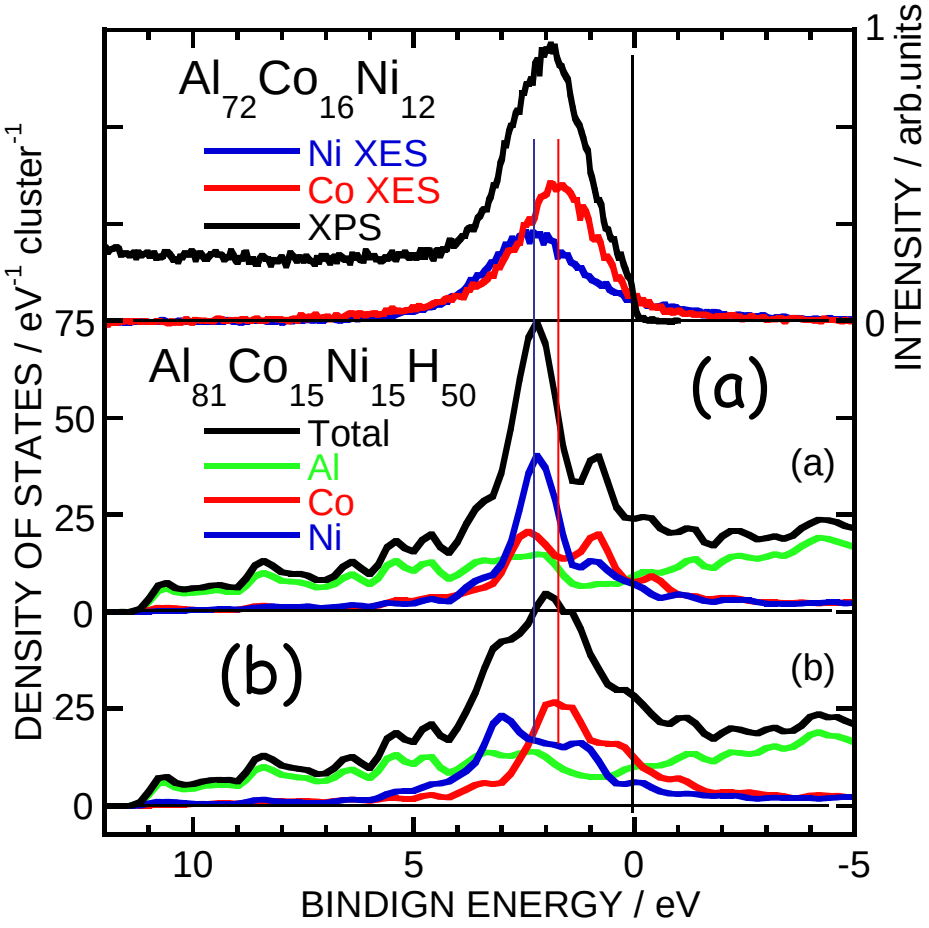
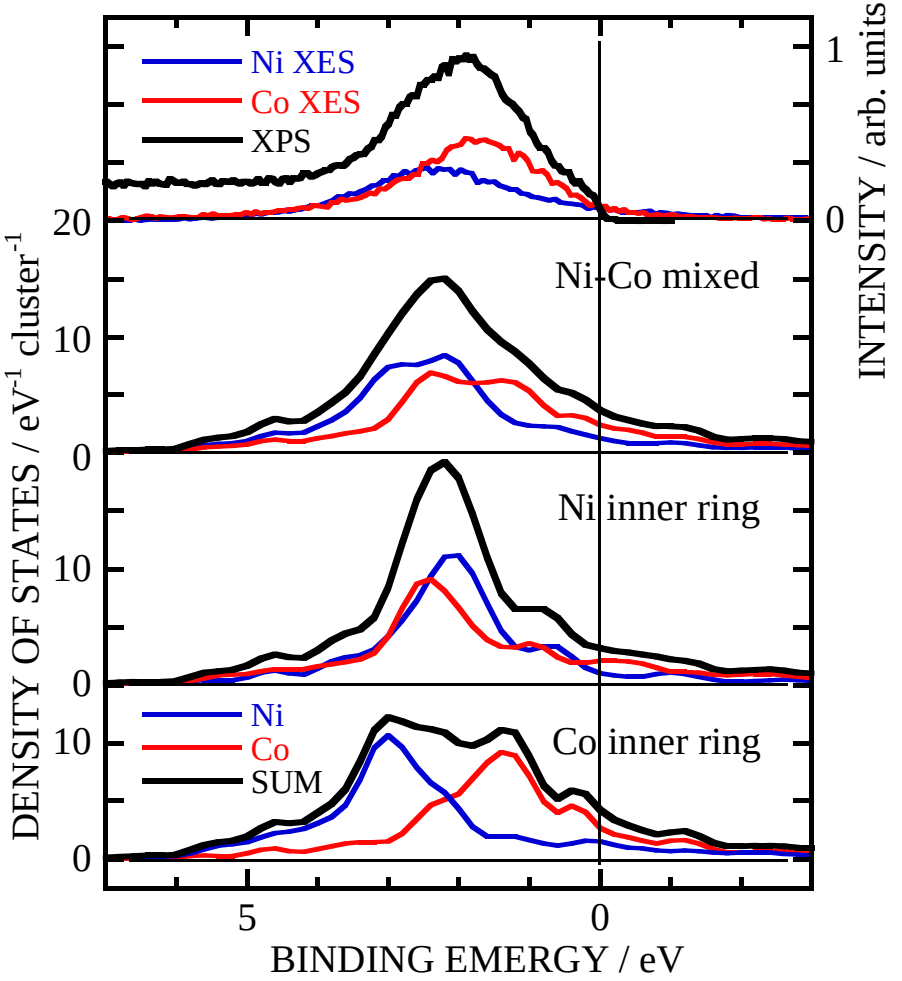
TM Arrangement

Al-Co-Ni



(a) Ni inner ring model
(b) Co inner ring model



Possible Co-Ni Mixing

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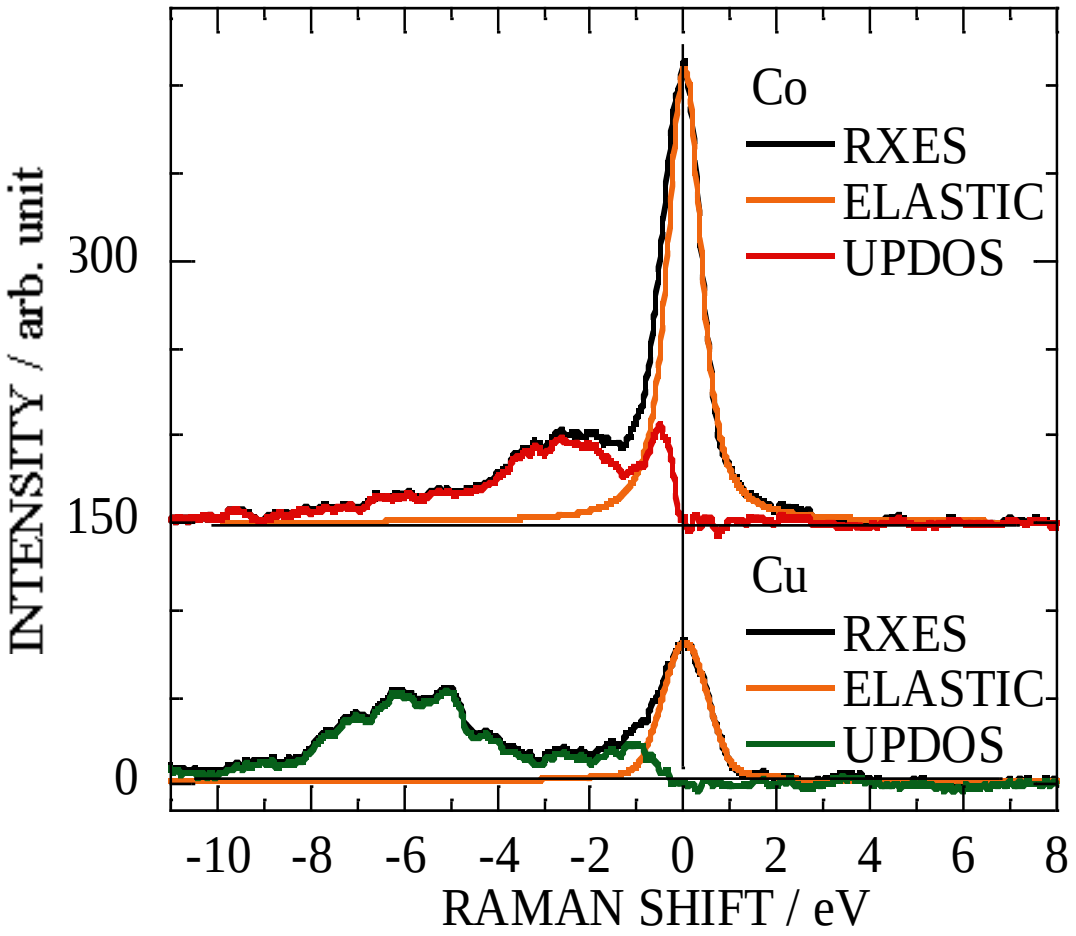
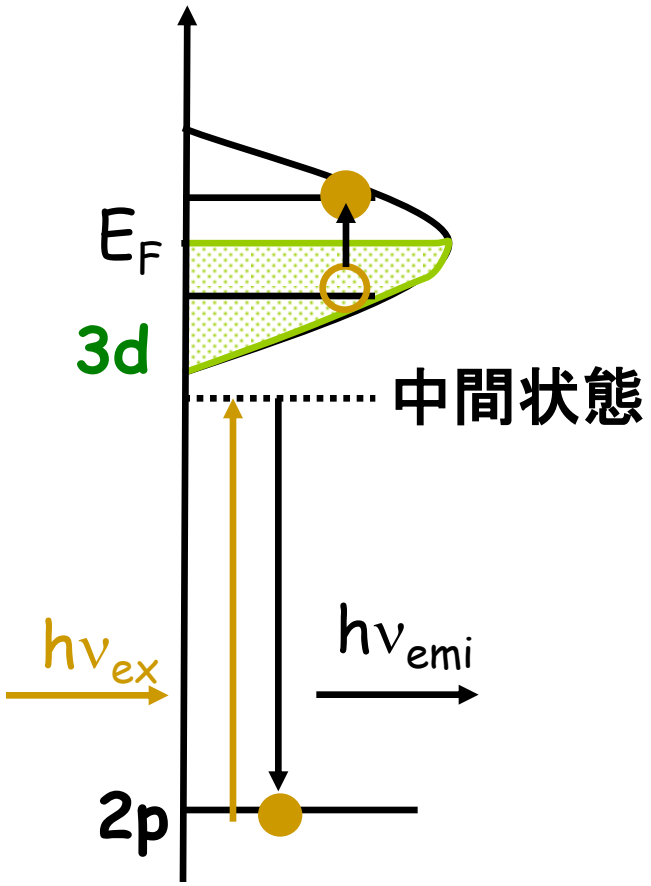
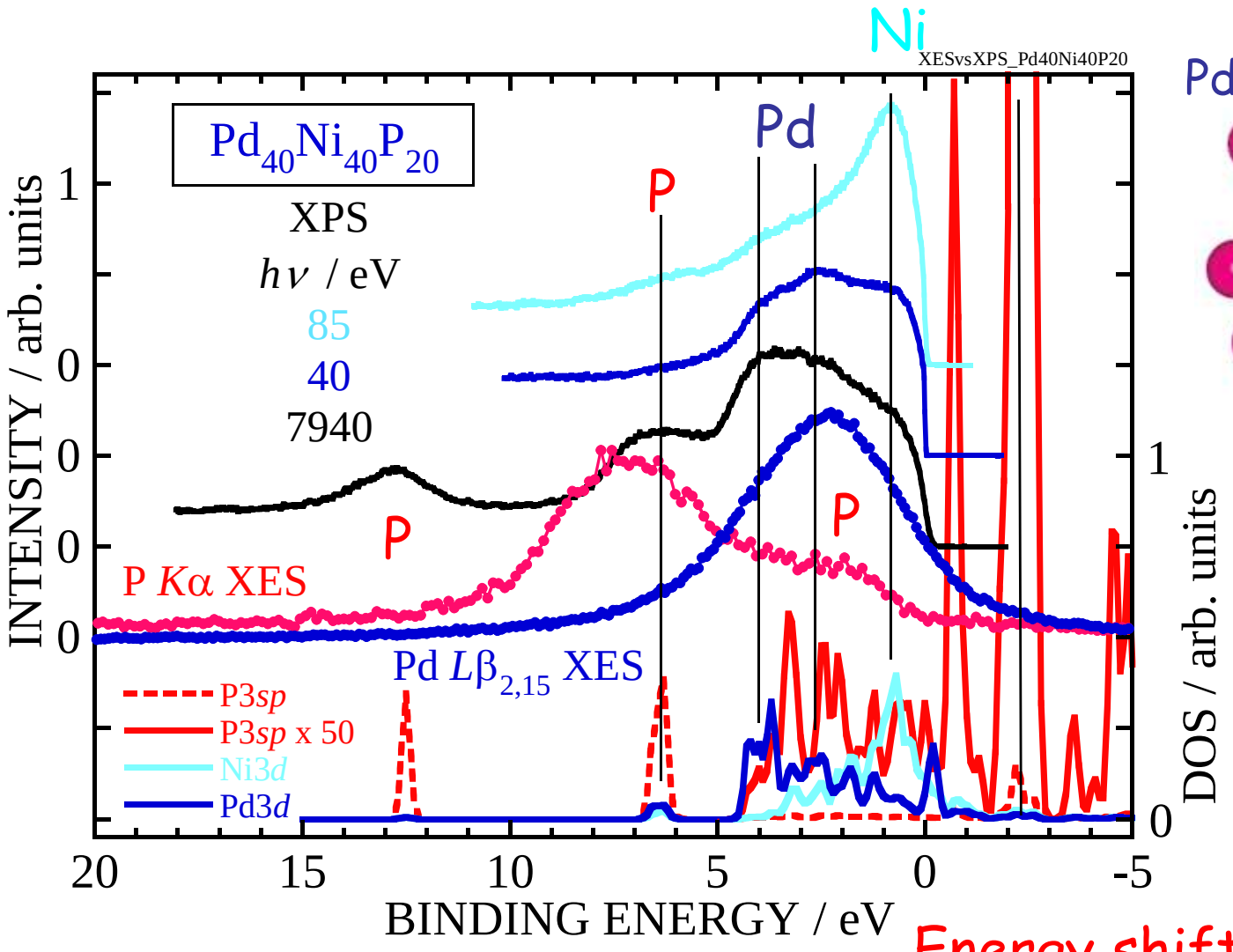
Raman Spectrum

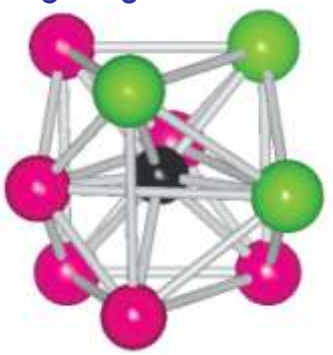
$Al_{65}Co_{20}Cu_{15}$





Valence-band Structure





Energy shift of P XES ?

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Microscopic Origin of High Structural Stability of BMG

Preferential Clusters [1]

- Chemical bond formation

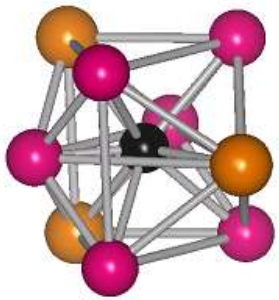
↓

Reducing U

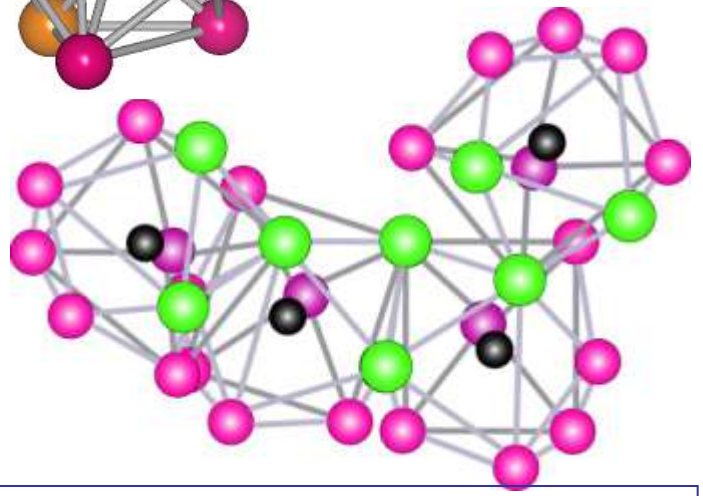
- Network Formation of Local Clusters

↓

Increasing S



Pd_3Ni_6P cluster
($PdNi_2P$ [2])



DOS of P ?
Pseudogap ?
金属性の強いZr-TM-Al系BMGの安定化機構は？

[1] C. Park *et. al.*, Mater. Trans. JIM, **40**, (1999) 491.
[2] M. Vennstörm, J. Höwing *et al.*, J. Solid. State. Chem., **177** (2004) 1449.

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Summary & Needs

Summary for QC

- TM 3d DOS > Co-Ni mixed arrangement
- Composition dependence ?
  decagonal ring in Co-rich phase and broken symmetry in Ni-rich one
- Psuedogap in Al DOS ? > Al *K* or *L* XES
- Unoccupied DOS in Resonant Raman ?

Summary for BMG

- Rigid local units + their flexible network formation
- Energy of P DOS ?
- Role of pseudogap (in more metallic Zr-BMG) ?

Needs

- *K*, *L* XES of light elements (Al, P etc.)
- Careful energy-calibration with XPS *et al.*
- High stability