

## FeNi インバー合金の局所構造

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1897年に Guillaume [1]によって発見されたインバー合金  $\text{Fe}_{65}\text{Ni}_{35}$  は、広い温度範囲にわたりほとんど熱膨張しない特徴を有し、多くの精密機械に利用されてきた。このインバー効果は、Fe の持つ磁氣的性質、すなわち、Fe には安定で原子サイズの大きな高スピン状態と、やや不安定でサイズの小さな低スピン状態が共存し、温度の上昇による通常の熱膨張と高→低スピン遷移による体積収縮が相殺するというモデル[2]で理解されてきた。

われわれは、蛍光 X 線ホログラフィー (XFH) 法を用いて Fe および Ni 元素のまわりで選択的に、3 次元的な原子イメージを構築した。その結果、Ni のまわりでは、X 線回折と同じ *fcc* 構造の原子イメージを見出したが、Fe のまわりでは、純粋 Fe と同じ *bcc* 構造的なイメージを見出した[3]。

本研究でわれわれは Fe および Ni *K* 吸収端付近で XAFS 測定を行うことにより、 $\text{Fe}_{65}\text{Ni}_{35}$  インバー合金の局所構造を詳しく探索することを試みた。その結果は、XFH の結果をほぼ追認していることを見出した。発表では、詳しくその結果を紹介する。

[1] C. E. Guillaume, *C. R. Hebd. Seances Acad. Sci.* **125**, 235 (1897).

[2] R. J. Weiss, *Proc. Phys. Soc. London* **82**, 281 (1963).

[3] S. Hosokawa et al., *SPring-8 Exp. Rep.* 2014B1187.

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### Abstract

Fe and Ni Ka x-ray fluorescence holography (XFH) measurements were performed on single crystal Fe<sub>65</sub>Ni<sub>35</sub> Invar alloy, which shows an extremely small thermal expansion coefficient over a wide temperature range [1], for investigating local atomic arrangement around each element. Around the Ni atoms, neighboring atoms are arranged to be a clear fcc lattice as obtained by x-ray diffraction. However, locally bcc-like atomic configurations are observed for the first- and second-neighboring atoms around the Fe element.

XAFS measurements were performed near the Fe and Ni K edges, and a peak are observed at the bcc position near only the Fe K edge. Thus, it is suggested that by cooling, an atom enters the bcc position near the Fe atoms, and the atoms at the fcc positions are positionally fluctuated in the angular directions. This would be the mechanism of the Invar effect and the high-spin low-spin transformation may be an additional phenomena.

[1] C. E. Guillaume, C. R. Hebd. Seanes Acad. Sci. 125, 235 (1897).

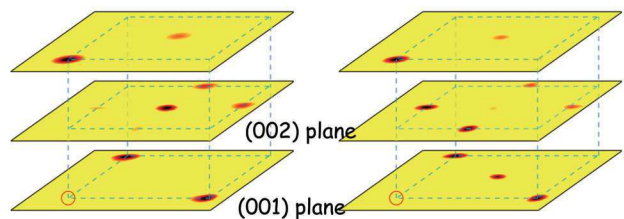
[2] R. J. Weiss, Proc. Phys. Soc. London 82, 281 (1963).

### Fe<sub>65</sub>Ni<sub>35</sub> Invar alloy



Lattice constant  
a = 3.58 Å  
crystal structure  
fcc

### Reconstructed images



Around Fe at 300 K

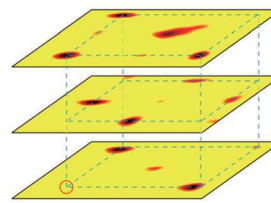
mixture of fcc and bcc structures



Clear fcc structure

Around Ni at 300 K

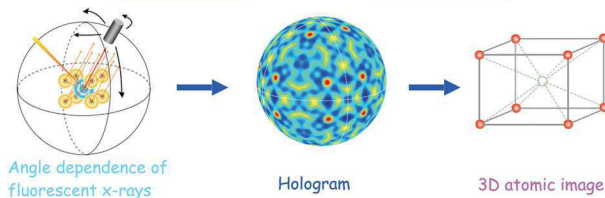
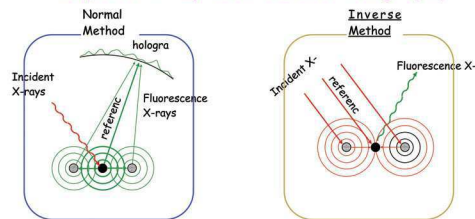
The atom images around Ni show fcc structure, the same as XRD



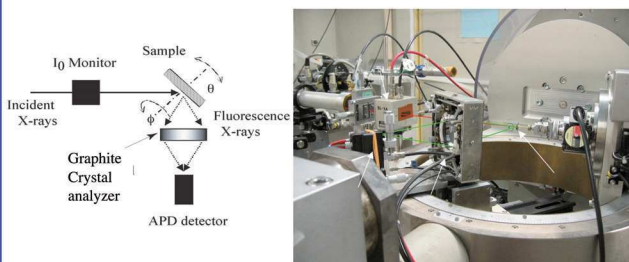
Around Fe at 100 K

The atom images around Fe atom show mixture of fcc and bcc structures at 300 K, while those show a clear fcc structure at 100 K

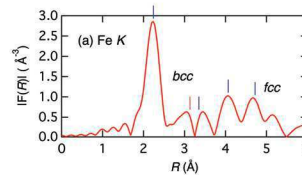
### Principle of x-ray fluorescence holography



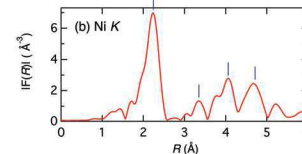
### XFH diffractometer installed at BL6C of PF-KEK



### XAFS data at 100 K

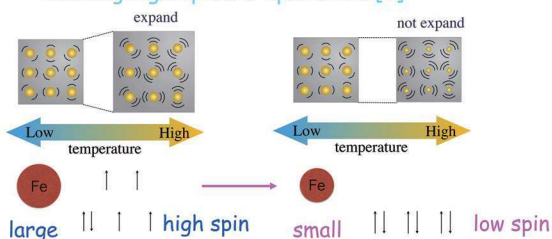


A peak appears at the bcc position around only Fe atoms



Purely fcc structures around the Ni atoms

### Existing high-spin low-spin model [2]



### Expected model

- By cooling, 1. An atom enters the bcc position near the Fe atoms
2. The atoms at fcc positions have positional fluctuation in the angular direction

