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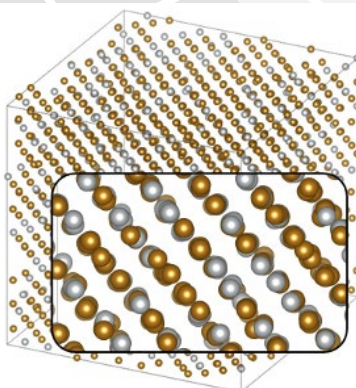
**2026.2.20 (Fri.) 16:30 ~**

### Venue: Meeting Room #486

Science Research Bldg. 1, 4th floor.  
Ehime Univ.

#### Keywords

1. Invar alloy
2. Magnetovolume effect
3. RMC modeling



# RMC modeling analysis of the large magnetovolume effects in Fe-Ni Invar alloys

Iron-nickel alloys with a disordered face-centered-cubic (fcc) structure are characterized by a ferromagnetic order with an expanded lattice due to the anomalously large magnetovolume effect ( $\omega_s$ ). The magnitude of  $\omega_s$  shows the maximum at a narrow composition range of  $\sim 35$  Ni at.%. The maximum  $\omega_s$  of  $\text{Fe}_{65}\text{Ni}_{35}$  gives rise to the large volume contraction with increasing temperature and reducing magnetization, which compensates the conventional thermal expansion and consequently results in zero-thermal expansion known as the Invar effect. In this talk, the atomic scale origin of the Invar effect and role of the large magnetovolume effects in the Fe-Ni alloys are discussed. For this purpose, we performed reverse Monte Carlo (RMC) modeling with a dataset of extended X-ray absorption fine structure and neutron total scattering. Our experiments revealed how the elongation of Fe-Fe bonds and larger atomic volume around Fe contribute to the Invar effect. The detailed analytical method using the reverse Monte Carlo method is also presented.