BL-9C/2025G033

Local thermal expansion of Co-containing Invar alloys II

Toshihiko YOKOYAMA[1,*], Hiromichi T. FUJII[2], Shingo MATSUMURA[2], and Naoki SAKAGUCHI[2]
[1] Institute for Molecular Science, Nishigo-naka 38, Myodaiji-cho, Okazaki, Aichi 444-8585, Japan
[2] Shinhokoku Material Corporation, 5-13-1 Arajuku-machi, Kawagoe, Saitama 350-1124, Japan

1 Introduction

Low thermal expansion materials are attractive from the viewpoints of both fundamental science and industrial technology. Previously we reported the results of Co-containing *fcc* stainless Invar alloy $Fe_{39}Co_{50}Cr_9Ni_2$ [1] developed by Fujii *et al*. [2] in Shinhoukoku Material Corp. It was found that Co exhibits a significant Invar effect as well as Fe, while the GX1Ni29-Co17 Kovar alloy $Fe_{53}Co_{17}Ni_{29}X_1$ does not. In the present EXAFS work, we have examined such Invar features by varying the Fe/Co composition ratio.

2 Methods

Two sets of the stainless Invar foils (10 μm thick) were prepared: $Fe_{39.0}Co_{49.9}Cr_{9.2}Ni_{1.9}$ (sample A) and $Fe_{37.8}Co_{51.3}Cr_{9.0}Ni_{1.9}$ (sample B). Both samples show *bcc* and *fcc* structures before and after annealing, respectively. Cr, Fe, and Co K-edge EXAFS spectra of *fcc* and *bcc* sample A and *fcc* sample B were recorded with the transmission mode in BL9C at 30-300 K.

To understand detailed mechanism of the thermal expansion, the path-integral effective classical potential (PIECP) Monte Carlo (MC) theoretical simulations have been also performed.

3 Results and Discussion

In the *bcc*-phase sample before annealing, no Invar effect was found by the dilatometric measurement; the lattice thermal expansion coefficient $\alpha_{lattice}$=8.61×10^{-6} (K^{-1}) at 200 K shows quite normal thermal expansion. The local thermal expansion obtained by EXAFS and PIECP agrees well with the macroscopic finding. In the EXAFS analysis, the first-nearest neighbor (NN) distance around Cr was found to be unnaturally longer than those around Fe and Co: R_{Cr}=2.510 Å, R_{Fe}=2.481 Å, and R_{Co}=2.474 Å. This result interestingly indicates that the lattice strain is concentrated in Cr, as in the case of stainless steel SUS304 [3] and SUS316L [4].

The dilatometric measurements of *fcc*-phase samples A and B reveal slightly positive thermal expansion in sample B at 100-200 K [$\alpha_{lattice}$=2.15×10^{-6} (K^{-1}) at 125 K], and much smaller thermal expansion in sample A [$\alpha_{lattice}$=0.37×10^{-6} (K^{-1})]. The EXAFS and PIECP results give more detailed information. Figure 1 shows the first-NN distances of sample A given by EXAFS; the EXAFS results give α_{Fe}=-0.931×10^{-6} (K^{-1}), α_{Co}=1.62×10^{-6} (K^{-1}), $\alpha_{Fe\text{-}Fe}$ =-2.36×10^{-6} (K^{-1}), $\alpha_{Fe\text{-}Co}$=0.179×10^{-6} (K^{-1}), and $\alpha_{Co\text{-}Co}$ =2.73×10^{-6} (K^{-1}) for sample A. This indicates that both Fe and Co participate in the Invar effect significantly, which reconfirms the previous work [1]. On the other hand, sample B provides α_{Fe}=1.15×10^{-6} (K^{-1}), α_{Co}= 6.98×10^{-6} (K^{-1}), $\alpha_{Fe\text{-}Fe}$ =-1.10×10^{-6} (K^{-1}), $\alpha_{Fe\text{-}Co}$= 4.71×10^{-6} (K^{-1}), and $\alpha_{Co\text{-}Co}$ =10.6×10^{-6} (K^{-1}). The invar effect in sample A is found to be more prominent in sample A. The PIECP results are also consistent with this observation at least qualitatively. The finding concerning local thermal expansion is nicely associated with the macroscopic thermal expansion feature. Since sample A contains a slightly more Fe/Co ratio, this consequence implies that the invar effect from Fe is more significant than from Co.

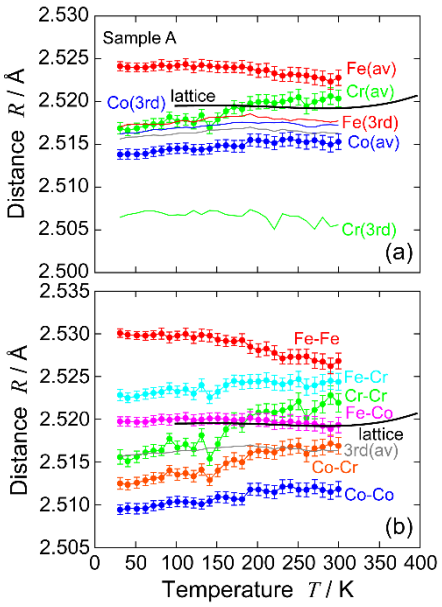

Fig. 1: Interatomic distances of *fcc* sample A. (a) average distances for the first-NN shells given directly by EXAFS, and (b) those for each atom pair estimated by the constant atomic radii model. The lattice thermal expansion is also shown. The third-NN distances (thin solid lines) are scaled by a factor of 1/√3.

References

[1] T. Yokoyama, H. T. Fujii, S. Matsumura, N. Sakaguchi, N. Kurahashi, and N. Maejima, *Phys. Rev. Materials*, **8** 083603 (2024).
[2] H. T. Fujii, N. Sakaguchi, K. Ona, F. Uraguchi, Y. Hayano, and T. Yokoyama, *Proc. SPIE*, *Advances in Optical and Mechanical Technologies for Telescopes and Instrumentation V*, 1218806 (2022).
[3] T. Yokoyama, A. Koide, and Y. Uemura, *Phys. Rev. Materials* **2**, 023601 (2018).
[4] T. Yokoyama and S. Chaveanghong, *Phys. Rev. Materials* **3**, 033607 (2019).

* yokoyama@ims.ac.jp