Local thermal expansions and lattice strains in Invar, Elinvar and stainless steel alloys

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Local structures and thermal expansions of alloys are often different from those from crystallographic expectations. Even when the x-ray diffraction patterns from the alloys are definitely observed, there should exist strains depending on the atom pairs and the local environments. In the present works, I will show element-specific local structures and thermal expansions of Invar ($Fe_{65}Ni_{35}$) [1], Elinvar (Ni Span C, $Fe_{49.66}Ni_{42.38}Cr_{5.49}Ti_{2.47}$), and SUS304 (AISI304, $Fe_{71.98}Ni_{9.07}Cr_{18.09}Mn_{0.86}$) [2] by the analysis of temperature dependent EXAFS concerning corresponding metal K edges and also by the Monte-Carlo (MC) simulations based on the path-integral effective classical potential (PIECP) method that includes the vibrational quantum effect approximately.

The alloy foils were purchased from Sugiyama Metals Co., Ltd. in Osaka, Japan. The thicknesses of Invar, Elinvar, and SUS304 are 10, 15.0, 10.5 μm, respectively. The Cr, Fe, and Ni K-edge EXAFS were recorded in BL9C of Photon Factory in High Energy Accelerator Research Organization (KEK-PF) with the transmission mode using Si(111) double crystal monochromator. The measurement temperatures were 10-300 K. The path-integral effective potential simulations for several kinds of alloy supercells of 500 atoms with periodic boundary restrictions were performed based on the NPT (constant number of particles, pressure, and temperature) conditions.

In the Invar alloy, the first nearest-neighbor (NN) shells around Fe show almost no thermal expansion, while those around Ni exhibit meaningful but smaller expansion than that of fcc Ni. At low temperature, the quantum effect is found to play an essentially important role. This is confirmed by comparing the quantum mechanical simulations to the classical ones, the latter of which exhibit large (normal) thermal expansion at low temperature. It is also revealed that thermal expansion for the Ni-Ni and Ni-Fe pairs is noticeably suppressed, even though the Ni electronic state may not vary depending on the temperature. On the other hand, the anharmonicity (asymmetric distribution) clearly exist for all the first NN shells as in the case of the normal thermal expansion system, where thermal expansion originates almost exclusively from the anharmonic interatomic potential.

From the analysis of the Elinvar alloy, the local thermal expansion around Fe is found to be considerably smaller than the ones around Ni and Cr. This observation can be understood simply because Fe in the Elinvar alloy exhibit an incomplete Invar-like effect. Moreover, in both the Elinvar and SUS304 alloys, the local thermal expansions and the lattice strains around Cr are found to be larger than those around Fe and Ni. From the PIECP MC simulations of both the alloys, the first-nearest neighbor Cr-Fe pair shows extraordinarily large thermal expansion, while the Cr-Cr pair exhibits quite small or even negative thermal expansion. These findings consequently indicate that the lattice strains in both the Elinvar and SUS304 alloys are

concentrated predominantly on the Cr atoms. Although the role of Cr in stainless steel has been known to inhibit corrosion by the formation of surface chromium oxide, the present investigation may interestingly suggest that the Cr atoms in the bulk play a hidden new role of absorbing inevitable lattice strains in the alloys.

[1] T. Yokoyama and K. Eguchi, *Phys. Rev. Lett.* **107**, 065901 (2011).
[2] T. Yokoyama, A. Koide, and Y. Uemura, to be published.