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

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1 Introduction

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.

2 Experiment

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 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.

3 Results and Discussion

The results of the Cr, Fe, and Ni K-edge EXAFS analysis concerning the first nearest-neighbor (NN) shells are depicted in Fig. 1. The local thermal expansion around Fe is found to be considerably smaller (1.33×10^{-5} Å/K) than the ones around Ni (2.17×10^{-5} Å/K) and Cr (2.32×10^{-5} Å/K). This observation can be understood simply because Fe in the Elinvar alloy exhibit an incomplete Invar effect. Here, the Invar effect indicates that the system consists of high-spin more stable Fe with larger atomic radius and low-spin more unstable Fe with smaller atomic radius and that as temperature increases enhancement of the low-spin Fe concentration yields thermal contraction, leading to compensation of thermal expansion due to anharmonic vibration. The SUS304 alloy exhibits normal thermal expansion as 2.85×10^{-5}, 2.39×10^{-5}, and 2.40×10^{-5} Å/K around Cr, Fe, and Ni. Moreover, it should be noted that in both the Elinvar and SUS304 alloys, the local thermal expansions and the lattice strains around Cr are 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 (figures not shown due to limited space). 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 stable and tight 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.

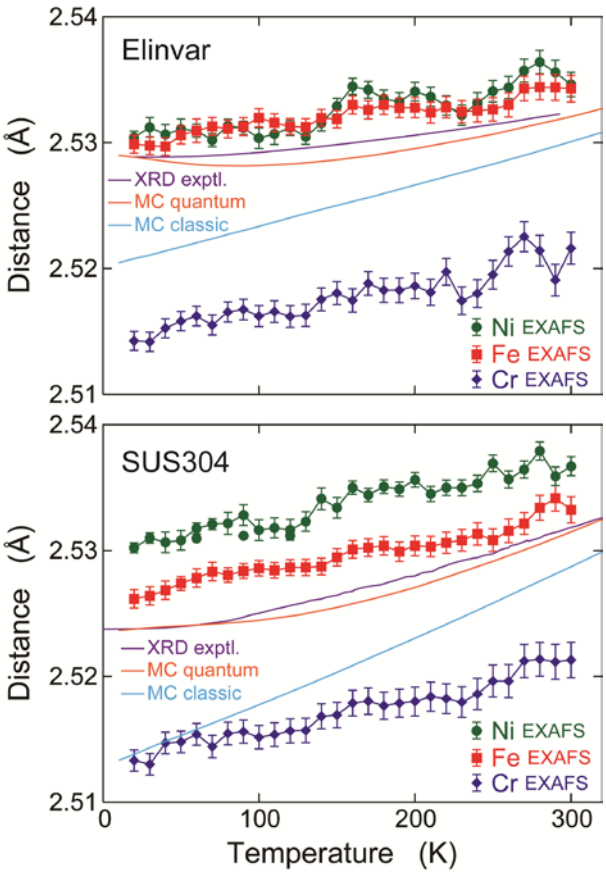

Fig. 1: Temperature dependence of the first-NN distances around Cr, Fe and Ni in the Elinvar and SUS304 alloys.

References

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