Surface Bain distortion

Shota ONO
Institute for Materials Research, Tohoku University, Sendai 980-8677, Japan

This project is motivated by the recent experiment of bending silver (Ag) nanowires [1]: the structural transformations from fcc to bcc to hcp to fcc structures are observed by bending the Ag nanowire. The fcc-bcc transformation has been explained by tetragonal Bain distortion [see Fig. 1(a)]. However, bcc Ag has been observed only near the surface [1]. In addition, bcc-structured fcc metals are known to be unstable at ambient condition. Therefore, the realization of bcc Ag is questionable.

In this project, we study the effect of surface on the Bain distortion. The DFT calculations are performed by using Quantum ESPRESSO, and the slab models are constructed by using Atomic Simulation Environment (ASE). Through the surface Bain distortion, fcc is transformed into "body-centered tetragonal (bct) structure", followed by a reoriented fcc structure [see Fig. 1(b)]. The bct phase is thermodynamically stable only when a fixed boundary condition is imposed, implying that such a metastable phase must be surrounded by fcc ground state [see Fig. 1(c)]. The present work has extended the Bain distortion concept to apply the surface systems and indicated that the surface could play an important role in phase transitions [2].

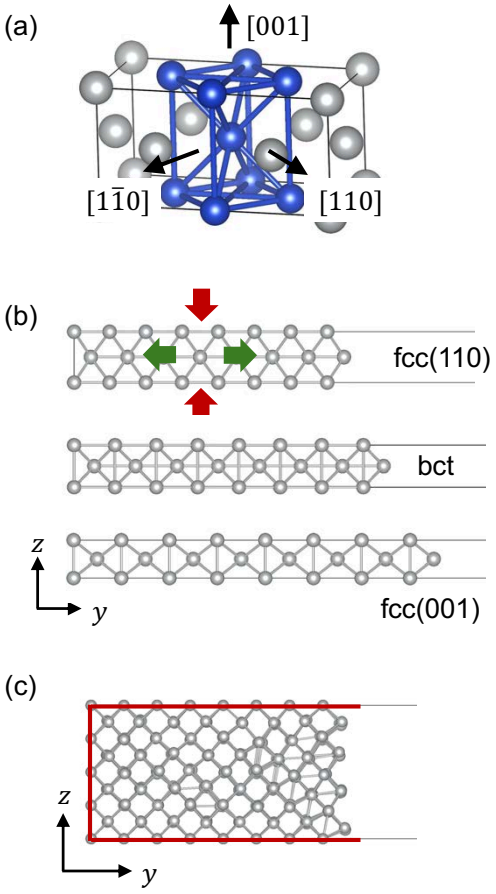

Figure 1: (a) Tetragonal unit cell in the fcc structure. A compression along the z-axis induces a transformation from fcc ($c/a = \sqrt{2}$) to bcc ($c/a = 1$) structure. (b) The surface Bain distortion of the Ag nanowire. The bct phase appears due to the free-boundary condition along the y-axis. (c) Atomic distribution of Ag nanowire in the bct phase after a molecular-dynamics simulation of 1.5 ps. Atoms on the boundary (red) are fixed during the simulation. Without the boundary condition, the bct phase is unstable [2].

References

[1] S. Sun *et al.*,: Phys. Rev. Lett. **128**, 015701 (2022).

[2] S. Ono and K. Tamura: Comp. Mater. Sci. **237**, 112920 (2024).