Lattice defect dynamics in harmonic structure metals through atomic simulations

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Core–shell harmonic structure materials, in which coarse grains (core regions) are surrounded by many fine grains (shell region), have excellent mechanical properties, particularly, the coexistence of high strength and ductility. In order to investigate the mechanism of the excellent mechanical properties, we use atomic and dislocation simulations. The harmonic structures are modeled simply while maintaining the three main characteristics of harmonic structure materials as shown in Fig. 1: heterogeneous distributed strength, interfaces between the core and shell regions, and shell region network. The results of the simulations[1)] show many synergistic effects of the coexistence of core and shell regions in the harmonic structure models as following: 1) Because the core region has lower strength than the shell region, the atomic simulations show that plastic deformation starts in the core region before the shell region. 2) The core–shell interface provides a strong resistance to dislocation transmission across the interface from the core region to the shell region. The dislocation simulations explain this resistance as a direct consequence of the back stress from the dislocations in the shell region. 3) Compared with the homogeneous structure model consisting of coarse grains with the same size of the core regions, the dislocation density of a portion of the core regions in contact with the core–shell interface increases, thus, the strength of the core region increases. 4) Compared with the homogeneous structure model with fine grains with the same size of the shell region, the strength of a portion of the shell network region in contact with the core–shell interface decreases. This weakening of the part of the shell network region is assumed to be due to the activation of plastic deformation by the stress concentration caused by dislocation pile-up in the core region.

The above results lead to a possible mechanism providing high strength and ductility in harmonic structure materials: 1) The high strength of the harmonic structure materials is provided by dislocation strengthening due to the core–shell interface in the core regions, which is sufficient to compensate for the weakening in the shell region. 2) The high ductility of the harmonic structure materials results from the suppression of plastic instability in the shell region, which is caused by the weakening of the shell region and the increased work-hardening rate of the core region because of the highly accumulated dislocations at the core–shell interface.

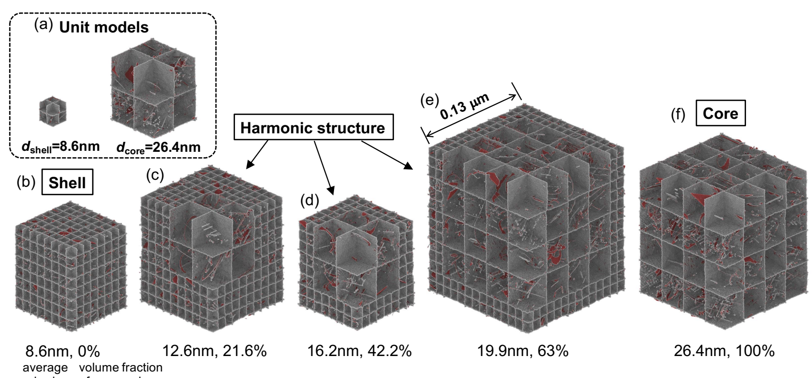

Fig. 1: Harmonic structure models constructed by two types of unit models with the grain sizes of 8.8 nm and 26.4 nm which correspond to shell and core regions.

1) T. Shimokawa, T. Hasegawa, K. Kiyota, T. Niiyama, K. Ameyama, *Acta Mater.* **2022**, *226*, 117679.