Elements Strategy Initiative for Structural Materials Director: Isao Tanaka (Kyoto University) Development of new structure materials based on new concept of plastic deformation process Research Project Outline for 3rd Phase (FY2018 to 2021)

Fundamental study on plaston concept and design principle of structural materials and structural

- ✓ Fundamental study of plaston on structure materials with variety of chemical bonding
- ✓ Design principles of structure materials

Development of novel structural materials through plaston concept

- ✓ Target 1 Development of novel steels with multiple plastron induced plasticity mechanisms
- ✓ Target 2 Development of titanium and titanium alloys with improved fatigue resistance
- ✓ Target 3 Collaborative works with new members oriented for materials processing

## **Research Results (FY2019)**

### Strategy for managing both high strength and large ductility in structural materials based on the concept of plaston

✓ Based on the concept of plaston, a strategy for overcoming the strength-ductility trade-off in metallic materials has been proposed in this project through combined efforts of materials processing, deformation mechanism analyses, atomic and first principles calculations. First comprehensive review

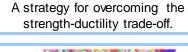
N. Tsuji, S. Ogata, H. Inui, I. Tanaka, K. Kishida, et al. Scripta Materialia (Viewpoint Article, Vol.181, 35-42 (2020)

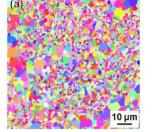
# Design principle of Mg alloy with large ductility

- ✓ Commercial Mg alloys (ZKX600) with a variety of mean grain sizes were fabricated by high pressure torsion (HPT) process. The plasticity-grain size relationship has been revealed.
- ✓ High strength and large ductility was successfully achieved in ultrafine grained materials. The plaston mechanism of the large ductility was found to be the activation the special dislocation slip having *c*-component, instead of deformation twin in large grained materials.

R. Zheng, T. Bhattacharjee, S. Gao, W. Gong, A. Shibata, T. Sasaki, K. Hono, N. Tsuji, Scientific Reports Vol.9 No.11702 (2019)

Principle for improving mechanical properties of Mg alloys

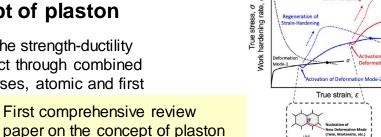




Commercial Mg alloy (mean grain size 0.77µm) fabricated by HPT



egeneration (



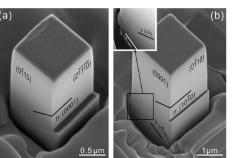
do/de

Regeneration of

### Plastic deformation of brittle materials with variety of chemical bonding

- ✓ Large plastic deformation was found by micro-pillar compression at room temperature in 6H-SiC which has strong covalent bonding and is usually regarded as a brittle material.
- ✓ Detailed deformation mechanism analysis found that prism slip together with basal slip occurs. Their critical resolved shear stress and atomic process have been revealed.

Design principles of brittle materials with improved plasticity



K. Kishida, Y. Shinkai, H. Inui, Acta Materialia, Vol.187, 19-28 (2020)

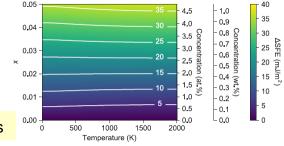
6H-SiC single crystal samples subjected to micro-pillar compression

#### Impact of interstitial C for stacking fault energy (SFE) of metallic alloys

✓ SFE plays a key role for plastic deformation of metallic materials. Using extensive sets of first principles calculations, impact of interstitial C in high entropy alloy CrMnFeCoNi has been revealed.

✓ Temperature dependence of SFE as well as the impact on the local environment of C have been evaluated.

Impact of interstitial C on plasticity of metals

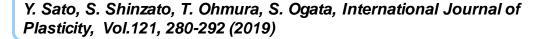


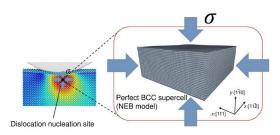
Y. Ikeda, I. Tanaka, J. Neugebauer, F. Körmann, Physical Review Materials, Vol. 3 113603 (2019) Dependence of C concentration and temperature on SFE in in high entropy alloy CrMnFeCoNi

#### Multi-scale simulation of nano-indentation process of BCC metallic crystals

- ✓ Nucleation process of plaston as experimentally observed pop-in during nano-indentation tests has been simulated via multi-scale methods.
- ✓ Temperature and strain-rate dependences of the plaston nucleation has been successfully predicted.

Matching of experiments and theoretical modelling for plaston nucleation





Stress state beneath the indenter onto BCC metallic crystals