【Grant-in-Aid for Scientific Research (S)】

Broad Section C

Title of Project : Nanomechanics on rewritable material strength by anomalous electrons

HIRAKATA Hiroyuki
(Kyoto University, Graduate School of Engineering, Professor)

Research Project Number: 20H05653　　Researcher Number : 40362454

Keyword : Material strength, Anomalous electrons, Mechanics of micro/nanomaterials, Nanomechanical experiments, First-principles analysis

【Purpose and Background of the Research】

For a long time, it has been believed that mechanical properties especially strength of materials are inherent to each material, that means, material constants are determined by the composition and microstructure of materials, and hence cannot be changed in principle. However, we found that the intrinsic strength of materials can be significantly altered by intentionally injecting excess electrons/holes, i.e., anomalous electrons, that cannot be present in nature (e.g., Fig. 1).

The purpose of this research project is to elucidate the fundamental mechanism of how anomalous electrons interfere with interatomic bonds and rewrite the strength and mechanical properties of various materials, and finally to establish a universal theory behind the exotic phenomena.

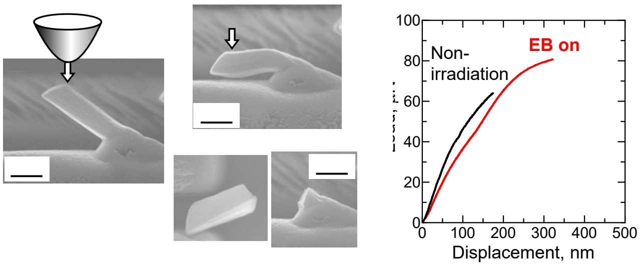

Figure 1 Effect of electrons on material strength

【Research Methods】

Plastic deformation and fracture are ultimately governed by the breaking of atomic bonds. To evaluate the ideal strength of materials that directly reflects the strength of interatomic bonds, we develop a series of experimental methods for nano/micromaterials without defects. In addition, we establish techniques for controlling (injecting, holding, and drawing) anomalous electrons in the material. By using these techniques, we conduct various experiments on electron-controlled specimens to elucidate the effects of anomalous electrons on material strength.

To understand the detailed transition of the bonding state by anomalous electrons and the accompanying change in deformation and fracture mechanisms from the viewpoint of quantum mechanics, we also perform first-principles strength simulations on materials with anomalous electrons. We systematically investigate the anomalous electron-induced strengthening characteristics for typical materials with covalent and ionic bonds via the development of the original theory (quantum-mechanics electronic stress theory) that decomposes and extracts the stress of each electron orbital and spin.

Based on the strength characteristics obtained by both the experiments and analyses, we elucidate the strengthening mechanisms by anomalous electrons and construct universal mechanical models.

【Expected Research Achievements and Scientific Significance】

-Elucidate the fundamental mechanism and principle of this anomalous phenomenon in which the macroscopic material strength can be changed by ultimately minute particles, i.e., electrons/holes.

-Propose rewritability that freely rewrites the material strength by controlling dynamic electrons. In other words, it brings conceptual innovation to material strength design from "making" materials to "drawing" functions.

-Establish the concept of basic evaluation technology for elucidating the effect of anomalous electrons on material strength.

-Extend the research field of anomalous electrons not only to mechanical properties but also to electric and magnetic properties and their multiphysics properties.

By realizing these, we will create a new scientific field for designing and creating a wide range of material functions.

【Publications Relevant to the Project】

・ Hiroyuki Hirakata, Kenta Konishi, Toshiyuki Kondo, Kohji Minoshima, Electron-beam enhanced creep deformation of amorphous silicon nano-cantilever, *Journal of Applied Physics*, Vol. **126**, 105102, 2019.

・ Hiroyuki Hirakata, Kyohei Sano, Takahiro Shimada, Electron-beam irradiation alters bond strength in zinc oxide single crystal, *Applied Physics Letters*, Vol. **116**, 111902, 2020.

【Term of Project】 FY2020-2024

【Budget Allocation】 154,800 Thousand Yen

【Homepage Address and Other Contact Information】

http://msr.me.kyoto-u.ac.jp