International Institute for Carbon-Neutral Energy Research

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Hydrogen Materials Compatibility Revised Roadmap

March 2019

KYUSHU UNIVERSITY

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ILLINOIS

Division Objective

- Provide the basic science that enables optimization of the cost, performance, and safety of pressurized hydrogen containment systems.
  - Development and use of advanced capabilities (experimental and modeling) to identify fundamental mechanisms of hydrogen-affected fatigue, fracture, friction and wear ~~and seizure~~ in materials
  - Development of predictive performance models for materials subjected to hydrogen-affected fatigue, fracture, friction and wear, ~~and seizure~~
  - Development of next-generation monolithic and functionally graded materials having lower cost and improved performance (e.g., higher strength) while retaining resistance to hydrogen-induced degradation.
  - Development of next-generation tribo-systems with higher efficiency and durability to save energy and reduce CO2 emissions.

Division Projects, Objectives, and Research Efforts (1)

Projects	Objectives	Research Efforts	Researchers
Project 1: Predictive Models of H_2-Assisted Cracking	Develop physics-informed, predictive models of H_2-assisted cracking in structural materials for technologically relevant loading conditions and temperatures	Establish comprehensive physical descriptions of H_2-assisted cracking at the proper size scales Establish relevant constitutive relationships for deformation in H_2-exposed materials Integrate physical descriptions and constitutive relationships into predictive model frameworks	Kubota, ~~Matsuda,~~ Kirchheim, Robertson, Sofronis, Somerday, Komoda, Aravas, Nagao, Ritchie Matsunaga
Project 2: Material Development for H_2 Service	Design cost-competitive materials for performance in H_2 service	Develop higher-strength, hydrogen-compatible stainless steels through advanced material processing methods Characterize and improve hydrogen compatibility of welds Develop and apply advanced surface coatings as hydrogen permeation barriers	Takaki, Kubota, Tsuchiyama, Yamabe, Macadre

Division Projects, Objectives, and Research Efforts (2)

Projects	Objectives	Research Efforts	Researchers
Project 3: Environmental Effects on Friction and Tribological Failures	Develop physics-based, comprehensive predictive models for friction and tribo-failures in order to improve reliability of tribological components in hydrogen-producing environments Develop physics-based, comprehensive predictive models for friction and wear in order to improve energy efficiency of machinery across technology sectors	Establish comprehensive description of mechanical and chemical processes at tribo-interface of metals, polymers, ceramics and coatings under sliding in H_2 Establish comprehensive description of hydrogen-assisted tribo-failure as well as methodologies to prevent hydrogen permeation and failure Establish comprehensive description of friction, wear, lubrication and surface failures in both dry and lubricated contact in various environment	Sugimura, Sawae, Tanaka, Yagi, Matsunaga, Morita, Yamaguchi, Saravanan, Niste

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Milestones (1)

Project 1: Predictive Models of H_2-Assisted Cracking

2014-2020 (short)

Establish validated physical description of contribution of *hydrogen-deformation interactions* to various cracking modes (Accomplished for intergranular and ransgranular cracking modes)

Establish validated physical descriptions of effects of *gas impurities* on H_2-assised cracking (Accomplished for O2 and CO impurities)

Establish relevant constitutive relationships for deformation in H_2-exposed materials subjected to different loading conditions and temperatures. Focus on single crystal Ni.

2021-2025 (mid)

Establish validated physical descriptions of H_2-assisted *fatigue crack initiation and propagation*

Establish validated physical descriptions of H_2-assisted cracking at *extreme temperatures*

Determine physics-informed criteria for H_2-assisted crack extension that are suitable for predictive models

2026-2030 (long)

Develop physics-informed, predictive models of H_2-assisted cracking under *cyclic loading* (fatigue)

Develop physics-informed, predictive models of H_2-assisted cracking under *static loading*

Develop physics-informed, predictive models of H_2-assisted cracking under *extreme-temperature conditions*

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Milestones (2)

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	2014-2020 (short)	2021-2025 (mid)	2026-2030 (long)
Project 2: Material Development for H_2 Service	Quantify fatigue limit in H_2 gas for austenitic stainless steel with *400 MPa yield strength*	Quantify fatigue limit in H_2 gas for austenitic stainless steel with *600 MPa yield strength* (Accomplished)	Quantify fatigue limit in H_2 gas for austenitic stainless steel with *800 MPa yield strength*
	Develop H_2-compatible, lower-cost austenitic stainless steels having *400 MPa yield strength* (Accomplished)	Develop H_2-compatible, lower-cost austenitic stainless steels having *600 MPa yield strength* (Accomplished)	Develop H_2-compatible, lower-cost austenitic stainless steels having *800 MPa yield strength*
	Develop and evaluate durable surface coating that resists hydrogen permeation at 100 MPa pressure (Accomplished)	Develop H_2-compatible welds for austenitic stainless steels (Accomplished: transferred to industry)	

Milestones (3)

	2014-2020 (short)	2021-2025 (mid)	2026-2030 (long)
Project 3: Environmental Effects on Friction and Tribological Failures	Establish physical description of salient factors and processes at tribo-interface of various candidate materials in H_2 (Accomplished: Identified governing factors for candidate materials)	Establish understanding of mechanical and chemical processes for friction and wear in H_2	Develop physics-based, mathematic models of friction and wear of various materials sliding in H_2
	Establish physical description of hydrogen generation, uptake, tribo-film formation and their relationship in lubricated rolling contact (Accomplished for typical synthetic oils and additives)	Develop a physics-based model of hydrogen-assisted tribo-failure under various lubricated conditions	Develop tribo-system to eliminate hydrogen-assisted tribo-failure.
	Establish physical description of effects of environment and surface modification of various materials in dry and lubricated contact (Accomplished for dry sliding of DLC and polymer composites and steel in boundary lubrication)	Develop physics-based mathematical models of friction, wear, lubrication and surface failure in both dry and lubricated contact in various environments	Develop tribo-system to optimize friction and/or to extend life by reducing wear and tribo-failure to improve energy efficiency of machinery

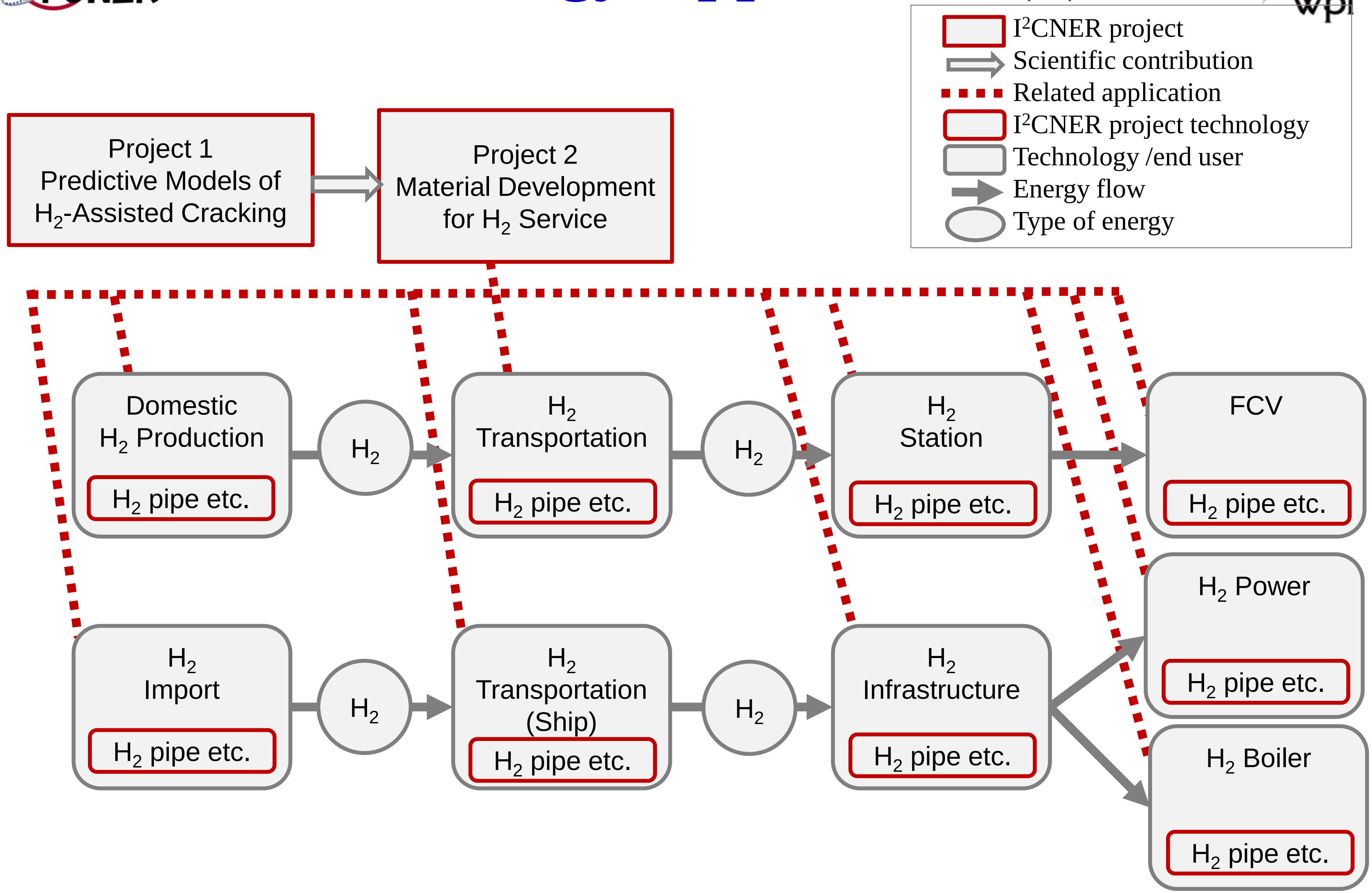
Ultimate Targets

	Ultimate targets	Current benchmark	Technology/ Application
Project 1: Predictive Models of H_2-Assisted Cracking	Physics-informed, predictive models that quantify H_2-assisted cracking as a function of material, environmental, and mechanical variables	Engineering models for quantifying component failure in H_2 service	Life prediction of H_2 containment components and material design for H_2 service Impurity research offers opportunities for the repurposing of existing non-hydrogen facilities for hydrogen use
Project 2: Material Development for H_2 Service	Materials designed specifically for high performance in hydrogen service	Adapting commercial materials (e.g. SUS316L stainless steel) for hydrogen service	Cost-effective, high-performance stainless steels for H_2 service including FCV, hydrogen station and hydrogen import system H2 compatible welds developed for HRS
Project 3: Environmental Effects on Friction and Tribological Failures	Physics-based predictive modeling approach for design and materials selection of tribological systems applied in a range of energy technologies	Empirical approach for design and materials selection of tribological systems in hydrogen and other service environments	High reliability tribological systems (e.g. valves and compressors in hydrogen infrastructure and rolling bearings in wind turbine gear box) Valves and compressor piston rings for high pressure H2 systems Reducing energy loss by improving friction components (e.g. in IC engines)

Role & Contribution through Technology

- **Role of this division toward CNS is to create**
  1. **low cost and higher strength stainless steel retaining resistance to hydrogen-induced degradation, underpinning the hydrogen economy**
  2. **low friction and wear components to reduce energy loss in various machinery and high-reliability tribological components to reduce tribological failure relating to increased severity in energy facilities such as wind turbines**

Technology/Application (1)



Technology/Application (2)