Ultrahigh-Flux Concerting Materials*)

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The purpose of the research unit UlCoMat (Ultrahigh-flux Concerting Materials) is creation of novel materials for advanced engineering systems, such as fusion and fission reactors, aerospace craft, rockets and chemical plants, based on understanding and control of the metastable phase and the self-organization induced in materials under extreme conditions. The UlCoMat will accelerate a paradigm shift from stable and resistant materials to metastable but adaptive ones. It focuses also on the science of life to seek long-life materials and a precise estimation of their existence for the development of robust engineering systems using the minimum materials compatible with economical and safety requirements.

Keywords: novel materials creation, metastable phase, self-organization, mesoscale structure, strength, physical property, metal, ceramic, composite

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1. Purpose of the Unit UlCoMat

The unit UlCoMat (Ultrahigh-flux Concerting Materials) is one of the eleven research units to be launched in April, 2023, at the National Institute for Fusion Science and the National Institutes of Natural Sciences, Japan [1]. The UlCoMat focuses on materials science for advanced engineering systems, including fusion reactors. Materials for fusion and other nuclear reactors, aerospace craft, rockets, chemical plants etc. are used under extreme conditions schematically depicted in Fig. 1. Fusion plasma, nuclear, jet and rocket fuels, chemical reduction-oxidation reactions, steam and other gas generation are extreme heat sources and also emit various radiations, leading to ultrahigh-flux energy and particles. The particles are, for example, neutrons, hydrogen isotopes and helium atoms in the case of plasma-facing blankets and divertors in fusion reactors. Generally, a single material cannot satisfy all the requirements of advanced engineering systems, therefore

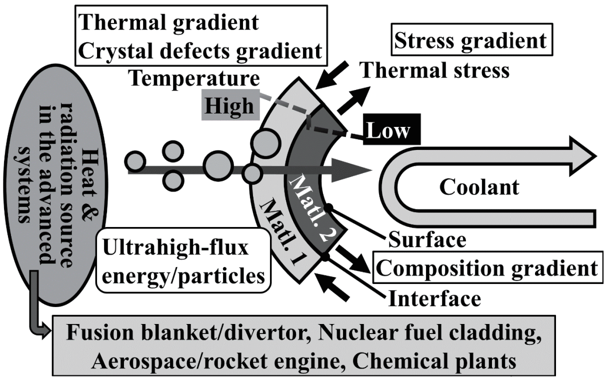

Fig. 1 Materials under extreme conditions including fusion environment with ultrahigh-flux energy and particles induced by various gradient fields.

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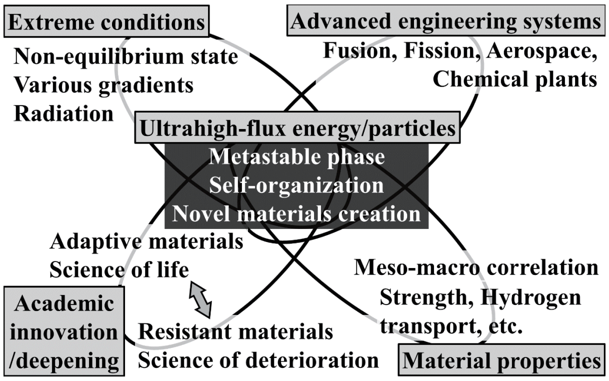

Fig. 2 Areas of focus by UlCoMat research unit.

dissimilar materials are combined as bonding, in other words, welding, coating and cladding, using Material (Matl.) 1 and Matl. 2 in the figure. The loading heat is eventually removed by a coolant to avoid the deterioration of strength and other functions at high temperature. In addition, the coolant transfers heat for energy conversion and power generation in the case of fusion and fission reactors. In other words, the systems are typically operated under severe one-sided heating conditions, where a steep gradient of temperature is induced and great thermal stress arises with a steep stress gradient, due to the mismatch of thermal expansions under constraint by bonding with each other. In the case of the fusion and fission reactors, high-dose neutron irradiation overlaps with severe one-sided heating and forms numerous crystal lattice defects in the materials, where defect-concentration can depend on a steep thermal gradient. Since chemical compositions are different among the materials including the coolant, the gradient of the element concentration is very steep at the interface of the bonding and at the surface to the coolant. It sometimes promotes atomic migration, resulting in formation of interlayer and corrosion products with different compositions. The advanced engineering systems are characterized by these steep gradients in various fields, promoting an ultrahigh flux of the constituent atoms in the materials.

Areas of focus of the UlCoMat are summarized in Fig. 2. A non-equilibrium state of materials is induced by ultrahigh-flux energy and particles under extreme conditions with multiplex steep gradients. The non-equilibrium condition causes amorphous and metastable compounds (metastable phases), and self-organization of constituent atoms, including crystal lattice defects. The purpose of the UlCoMat is creation of novel materials for advanced engineering systems, based on understanding and control of the metastable phase and self-organization in materials. Especially for self-organization, periodic patterns with an interval of several tens of nanometers to microns have been identified, even in solid matter under a large deformation [2, 3], neutron and ion-irradiation conditions [4, 5], as shown in Figs. 3 and 4 for example. These mesoscale pattern formations have been well classified and simulated based on numerical analyses [6, 7]. However, their physics are still incomplete, novel, and it is very interesting to reveal how they induce the macroscopic properties of materials, such as strength, an irradiation response, hydrogen-isotope transport, corrosion and so on. The understanding of the physics enables us, for materials design, to accelerate adaptive structures concerting with an ultrahigh flux of energy and various particles. Such ultrahigh-flux concert-

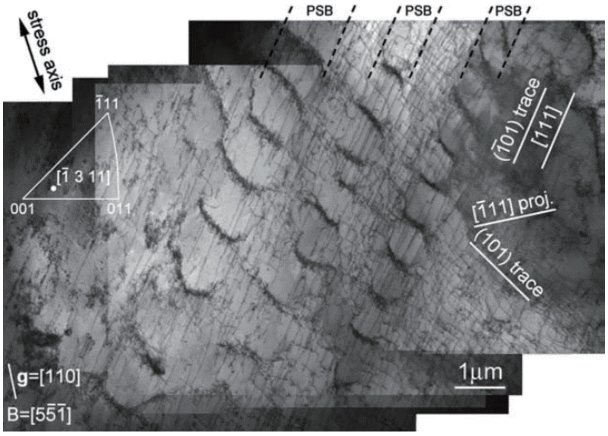

Fig. 3 Periodic dislocation ladder structure at persistent slip bands (PSBs) in ferritic steel X10CrAl24 after fatigue test with 0.2% in plastic strain amplitude for 9000 times at room temperature. Ladder patterns consist of high and low density of dislocations in PSB area. Dislocations striated crystal lattice defects, appear as dark contrast lines in picture. Heavy fatigue deformation induced dislocation motion and interactions, leading to self-organization as ladder patterns. Reprinted from ref. [3] with permission.

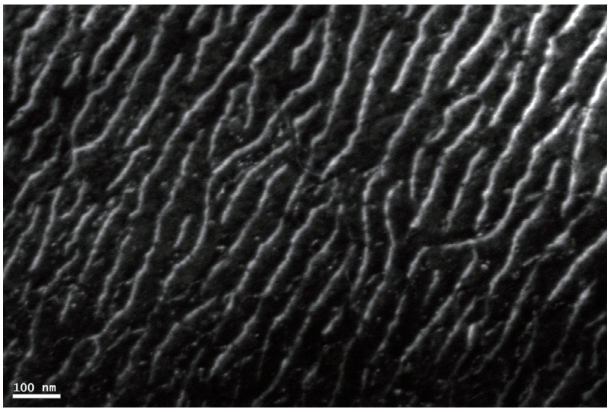

Fig. 4 Stripe patterns of defect clusters in 12Cr ferritic steel irradiated by Kr ions up to 15 dpa (displacement per atom) at 20°C. White contrast lines consist of defects clusters, considered as interstitial atoms, produced due to ion-irradiation-induced displacement of lattice position atoms. Interstitial atom clusters observed as white dots at formation, then migrated, finally aligned as bold white stripes due to self-organization. Reprinted from ref. [5] with permission.

ing materials will make an academic innovation through a paradigm shift from stable and resistant materials to metastable but adaptive novel materials. On the other hand, perfect adaptation is absolutely unrealistic, because materials degradation is unavoidable if the adaption is less than enough for perturbation of the extreme conditions, accumulation and intrinsic mutation of materials damage structure. The UlCoMat also focuses on unavoidable materials damage, based on an understanding of the reversibility and irreversibility of microstructural and macroscopic properties. Based on these physics, the UlCoMat also seeks long life materials and a precise estimation of their lifespans to develop robust engineering systems, using the minimum materials compatible with economical and safety requirements. In other words, an academic deepening of the science of materials' lifespans and their controllability is also an important focus to break away from the conventional materials science of deterioration.

2. A Hopeful Sign for Ultrahigh-Flux Concerting Materials

Fusion reactor materials for a plasma-facing blanket first wall are expected to be irradiated with intense neutron irradiation up to 100 dpa (displacement per atom), which is equivalent to a dose of nearly 10^{27} neutrons/m^2 with 14 MeV in neutron energy [8]. Neutron irradiation swelling is one of important issues for development of fusion reactor materials and also other nuclear reactors, because volume changes by the swelling cause yielding stress, which confine the materials into the original volume in the components. The typical acceptable limit of swelling is 2% for the structural materials in ITER, an experimental fusion reactor [9]. Neutron irradiation swelling becomes considerable around $0.4T_m$, where T_m is the melting point of base metal. The swelling is usually increased monotonically with an increasing neutron irradiation dose up to several tens to 100 dpa [10]. On the other hand, some vanadium alloys have exhibited abnormal swelling behavior, as shown in Fig. 5 [11]. These swelling curves showed peaks with 1.5 to 2% in the density change at 40 to 70 dpa, then decreased to less than 0.5% at over 110 dpa. It has been found that the decrease in the swelling was synchronized with the formation of a metastable phase Ti_5Si_3 [12]. Ti_5Si_3 is an irradiation-induced non-equilibrium phase and never appears under a thermal equilibrium state of the V-Cr-Ti alloy system containing around 0.1 mass% or less of Si as an impurity. Similar behavior with a swelling peak at 30 dpa, then a decrease at over 50 dpa has been observed for stainless steels irradiated with neutrons at 500°C [13]. In this case, irradiation-induced MC type carbide precipitation was synchronized with the decrease in swelling. The mechanisms for these abnormal swelling behaviors have not been revealed yet, however the interface between the metastable phase precipitates and the alloy matrix likely acted as sink for the radiation defects. They were able to change the sink balance, and eliminate vacancy clusters smaller than a critical size for unstable growth of the voids, leading to considerable swelling. Based on these phenomena, it is possible to recover the swelling if we understand the mechanisms for the formation of the metastable phase and control their precipitation during heavy irradiation by, for example, optimization of the composition and microstructure before irradiation. Such self-recovery behavior by dynamic control of the microstructures will extend the materials lifespan very much. Especially, the metastable phase and self-organization will be a key to creation of the ultrahigh-flux concerting and thus long-life materials.

3. Strategy for Materials Research

Based on the scientific background of the starting members of the UlCoMat, the research targets are recognized as indicated in Fig. 6. The materials to be investigated are categorized into structural materials and functional ones. The structural materials consist of metals and ceramics. The metallic materials for investigations are (1) refractory metals, where their covalent bond is relatively larger than the other metals, and therefore good high-temperature strength is expected, as with ceramics, and (2) non-refractory metals strengthened by dispersion

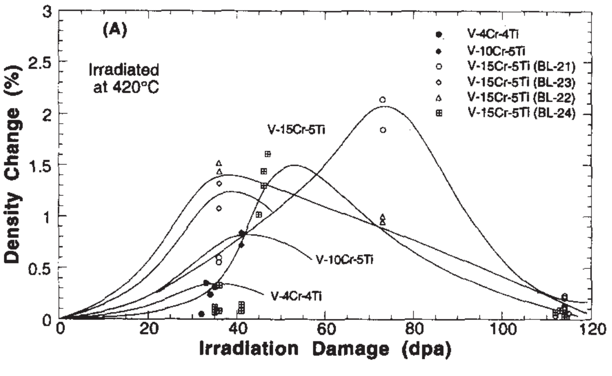

Fig. 5 Neutron irradiation swelling of vanadium alloys at 420°C. Reprinted from ref. [11] with permission.

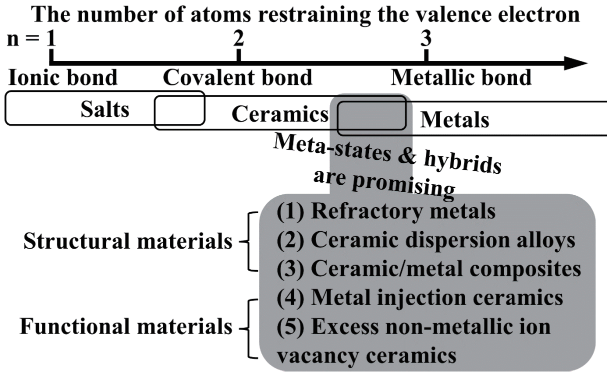

Fig. 6 Meta-states and hybrids in classification of solids.

of refractory ceramic nano-particles. On the other hand, (3) brittle ceramic materials are to be modified for metallic pseudo-ductility etc. by extrafine fibrillization, joining and composite assembly with metallic materials. The fusion materials community, including the members of UlCoMat, have already various achievements with these materials, such as tungsten [14] and vanadium alloys [15] for the topic (1) of refractory metals, oxide-dispersion-strengthened steels [16, 17] for (2), and SiC/SiC composite [18, 19] for (3). Especially the achieved material technologies for high-temperature strength are believed to be spreadable to other advanced engineering systems. Besides, ceramic functional materials are to be improved by (4) metallic injection/dispersion and (5) introduction of supersaturated non-metallic ion vacancy defects and accompanied metallic bonding. In the field of fusion applications, deterioration of ceramic properties for an insulator and hydrogen permeation barrier have been mainly discussed with respect to the topics (4) and (5) [20, 21]. However, such deterioration can be applied for conductive ceramics and a super-permeation membrane [22], respectively, as new functions of meta-state materials. The deterioration for fusion application and new characteristics for other fields are two sides of the same coin for functional materials research.

In conclusion, both the structural and functional materials research of UlCoMat can extend to interdisciplinary areas, based on past achievements and ongoing changes from the standpoint of promising meta-state and hybrid materials, namely, ceramic metals and metallic ceramics.

4. Summary

Extreme conditions, including a fusion environment, are characterized by an ultrahigh flux of energy and particles with steep gradients and radiation damage. They induce a non-equilibrium state, forming a metastable phase and self-organization in materials. The research unit UlCoMat focuses on (1) how the non-equilibrium phase induces macroscopic properties, (2) materials design for adaptive structures concerting ultrahigh flux, (3) a paradigm shift from stable and resistant materials to metastable but adaptive materials, and (4) a science of materials' lifespans for robust engineering systems, using the minimum materials compatible with economical and safety requirements. The strategic investigation targets are meta-state and hybrid materials, such as ceramic metals and metallic ceramics.

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