材料機能・信頼性設計評価研究部門　Division of Design and Evaluation of Function and Reliability of Materials

ナノ界面機能・信頼性設計学研究分野
Laboratory for Functional Design of Nano-Scale Interface

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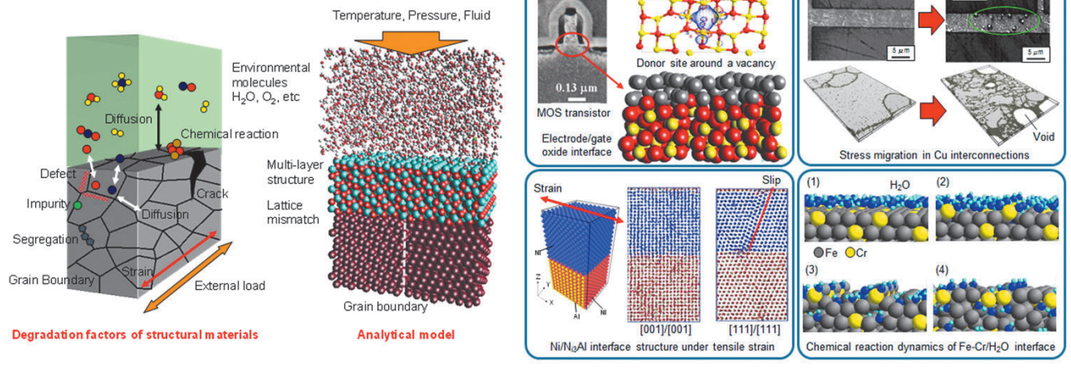
持続発展可能な社会の実現に向けて、ナノスケールの電子デバイスから発電プラントのような巨大構造体に至るまで、機器を構成する材料システムの高機能、高性能、長寿命化が求められている。これまで新材料の開発や複合化、微細化などによりこれら目標は達成されてきたが、その反面、材料システムは複雑化し、組織の不均一性や不安定性は増大する傾向にある。特に積層構造体や複合材料における異種材料界面では、濃度勾配やひずみ勾配が存在するため使用条件や使用環境によって界面組織が時間とともに変化し、この組織変化を起因とする不良や損傷が顕在化してきた。そこで、材料界面の組織変化発現メカニズムを材料、環境、力学の相互作用の観点から原子レベルシミュレーションにより明らかにし、異種材料界面組織変動メカニズムに立脚した高機能・高信頼材料の設計開発研究を推進する。

We have been conducting investigations of the interface integrity in various material systems such as nano-scale semiconductor devices, fuel cells, batteries, structural materials used for power plants. These complex material systems have the disordered atomic configuration in a thermodynamically metastable structure near a heterogeneous interface and then, the gradient of composition and strain always exists around the interface. Therefore the interface structure changes with time due to the gradient and thus, both the various properties reliability of the material system deteriorate easily. From this point of view, in order to design the interface integrity for ensuring the reliability of material systems, dominant factors cause the change in the interface structure under stress or strain are determined by using computational simulations and experimental methods. In addition, we are going to develop a method for analyzing the fluctuation of physical properties caused by atomic-scale damage and defects based on electronic- and atomic-level computational simulation techniques.



Explicating the fluctuation mechanism and design of the functional interface integrity based on atomic-scale simulations

原子レベルシミュレーションによる材料界面健全性評価と信頼性設計
Design of the functional interface integrity based on atomic-scale simulations

多種多様な材料が集積された複合材料システムの性能, 機能向上や安全性・信頼性の向上を目的に、原子レベルシミュレーションを用いて、異種材料界面近傍のひずみ（応力）、組成、格子欠陥（空孔、格子間原子や不純物）の相互作用による組織変化メカニズムを解明する。これによって異種材料界面構造安定化の支配因子を明らかにし、次世代エネルギー・環境インフラに資する複合材料システムの高性能化と長期信頼性を確保するため、界面構造の安定化を目的とした界面組織の設計と試作評価を通した実証研究を推進する。

The aim of this research is to explicate dominant factors for improving the interface integrity in material systems. Atomic-scale simulations such as quantum chemical molecular dynamics are applied for the analysis. The mechanism of the change in the structure of the interface between stacked thin-films, precipitate/matrix interface and metal/environment interface has been studied by focusing on the strain-induced and accelerated atomic diffusion. To improve the performance and reliability of the macro and nano scale products and devices, we have been developing methods for optimizing the interface structure, material, and fabrication process.

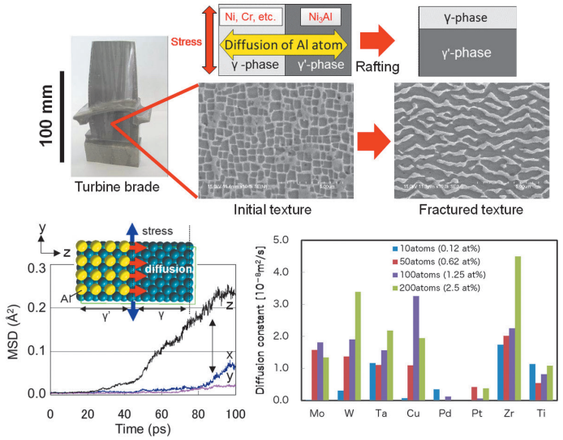


Fig.1 Explication of the fracture mechanisms of Ni-base superalloys at high temperatures under creep conditions by considering stress-induced anisotropic diffusion of component elements and effects of alloying element on the diffusion

異種材料界面組織, 物性変動メカニズム評価手法の開発
Development of analytical methods for explicating the fluctuation mechanism of the interface structure and material properties

様々な材料系に存在する異種材料界面の組織変動、物性変動メカニズムを解明するため量子力学に基づく解析技術を開発する。これにより、組成や結晶構造、物性が不連続な異種材料界面における原子結合状態と電子状態を解析し、各材料の原子レベル構造変化と各種物性（強度、電気伝導特性）の変動メカニズムを明らかにする。また、ナノ、マイクロレベルの組織観察や強度試験を実施し、解析結果の妥当性を検証することでその高度化を進め、理論と実験の両輪からなる材料設計・評価の学術基盤の構築を目指す。

The aim of this research is to develop new quantum mechanics based computational simulation methods for explicating the fluctuation mechanism of the interface structure and material properties. The influence of atomic and electronic structures of the heterogeneous interface on physical and chemical properties of material systems such as strength, corrosion resistance, thermal and electrical conductivity is discussed. In order to validate the analytical results and improve the simulation accuracy, the change in these properties are measured by using micro- and nano-scale measurement methods. We are going to develop a method for optimizing interface structure by the combination of computational simulation and experimental analysis.

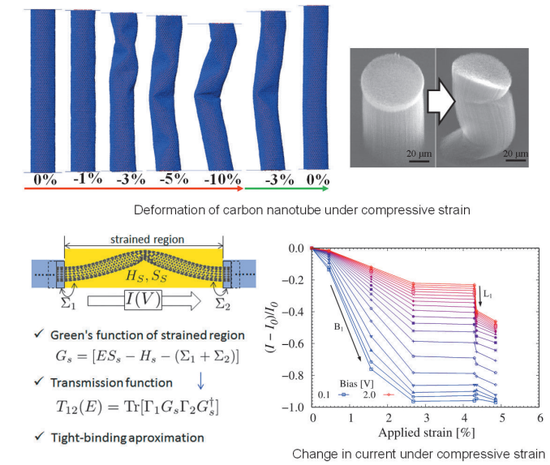


Fig.2 Development of a new method for analyzing electron transport properties using tight-binding based Green's function method and its application to estimate current though carbon nanotube under uniaxial compressive strain