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研究課題名（和文）Modeling of ductile failure in multi-phase metallic materials

研究課題名（英文）Modeling of ductile failure in multi-phase metallic materials

研究代表者

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研究成果の概要（和文）：結晶塑性有限要素法を用いて、多相材料の破壊に至るまでの機械的応答を予測する方法を提案した。我々は、統計的手法による多相材料のモデリングのための新しいアプローチを開発した。損傷の発生と進展を考慮した非局所的な結晶塑性モデルを開発した。損傷モデルパラメータの正確なキャリブレーションのために、実験的に観測されたボイドの局所応力-ひずみ曲線の抽出に基づく新しい手順を提案した。さまざまなミクロ構造を持つ複数の二相鋼に対して検証した。推定された破壊位置が、異なる微細構造に対して類似していることが判明し、このことから類似した固有特性が示唆されるとともに、キャリブレーション手順の頑健性も確認できた。

研究成果の学術的意義や社会的意義
The proposed framework is general and modular, and is applicable to a wide variety of materials. By carefully calibrating the model, it is also possible to predict the behavior of other materials without experimental testing and thus accelerating the development of alloys with improved properties.

研究成果の概要（英文）：In this research, a method for predicting the mechanical response of multi-phase material up-to-failure was proposed using the crystal plasticity finite element method. We developed a new approach for the modeling of mutli-phase materials by statistical means. A non-local crystal plasticity model taking into account damage initiation and evolution was developed. A new procedure based on the extraction of the local stress-strain path of experimentally observed void was proposed for the accurate calibration of the damage model parameters. The approach was tested against multiple dual-phase steels with varying microstructures. The estimated fracture loci were found to be similar for the different microstructures suggesting similar intrinsic properties and confirming the robustness of the calibration procedure.

研究分野：Micromechanics

キーワード：Crystal plasticity　Finite Element Method　Dual-phase steels　X-CT　Ductile failure

１．研究開始当初の背景

The development of new structural materials with improved properties is a perpetual pursuit in materials science. In particular, the increasing demand for lightweight structures request the development of alloys having both high strength and high ductility to overcome the so-called strength-ductility trade-off. Among the vast family of metallic alloys, multi-phase materials, such as dual-phase (DP) steels, duplex α/β titanium alloys or Mg/LPSO two-phase alloys often consisting in a blend of soft/ductile and hard/brittle phases are of particular interest as their performances are directly related to the individual phase's properties, their morphologies, distributions, and volume fractions.

However, the exhaustive exploration of available microstructural space by experimental trial-and-error approaches is not feasible in a timely and inexpensive manner. Alternatively, the virtual exploration of the design space through Integrated Computational Materials Engineering (ICME) approaches using for instance the Crystal Plasticity Finite Element Method (CPFEM) has become attractive due to the improvement in computational performances and the increased availability of a wide panel of open-source software and tools. Through the explicit representation of a polycrystal accounting for key microstructural attributes (grain size, texture, phase distribution), the CPFEM is efficient at predicting the macroscopic response of the aggregate prior to damage onset. However, the development of damage-tolerant materials requires the prediction of the mechanical behavior up-to-failure and thus the constitutive model should account for the onset of damage and its evolution at the local scale. In addition, damage models are generally calibrated based on the macroscopic response of the material in terms of stress-strain or load-displacement curves. This method is suitable for structure-oriented models but not for microstructure-sensitive ones since the local micromechanical fields at void sites may significantly differ from the macroscopic ones. Accordingly, new calibration procedures based on micromechanical experimental data should be proposed.

２．研究の目的

The main objective of this research was to develop a microstructure-oriented numerical framework for the prediction of the complete mechanical response of multi-phase materials up-to-failure. The proposed framework, centered around the CPFEM, would specifically focus on (1) developing new methods for the realistic representation of multi-phase polycrystalline aggregates (2) developing a robust crystal plasticity model including damage initiation and evolution and (3) calibration and validating the model from experimental data.

３．研究の方法

<Statistical and spatially resolved modeling of multi-phase polycrystalline materials>

Microstructural observations were carried out by scanning electron microscopy (SEM) and electron backscattered diffraction (EBSD) measurements to statistically quantify both key microstructural features (grain size, shape, spatial distribution of phases) and crystallographic texture (local orientation, misorientation, specific orientations relationship…), notably through the usage of the orientation distribution function (ODF). As an accurate prediction requires the modeling of a representative volume element (RVE) that catches key microstructural features. In literature, it is often achieved using the so-called Voronoi tessellation even though it suffers from significant drawbacks such as the lack of control of grain size and shape. In recent years, the applicant has developed an anisotropic tessellation based on the random filling of a domain with ellipsoids allowing the generation of synthetic microstructures with controlled grain size and shape. However, in the case of multi-phase materials, the spatial distribution of phases is a key parameter to include. Therefore, a method was proposed based on the experimentally estimated spatial correlation functions, to carefully control the positioning of the different phases within the RVE.

<Development of a robust crystal plasticity/damage model>

In classic ductile fracture theory, damage is generally described as the progressive process of void nucleation, growth, and coalescence. This theory has been extensively applied in isotropic continuum damage mechanics. In particular, the Gurson model based on a modification of the J2 yield criterion has received extensive applications. However, these models are structure-oriented and do not consider local micro-mechanical fields at the microstructure scale. On the opposite, most anisotropic crystal plasticity models do not explicitly account for damage mechanisms at the crystal scale. Therefore, a constitutive model combining both crystal plasticity and damage formation was developed. Damage was considered through the introduction of a void volume fraction Φ and on the application of the "effective stress" concept to account for the local stiffness degradation. The evolution of the void fraction was described based on relevant micro-mechanical fields (local plastic strain, local triaxial stress state…). The model was written as a UMAT for the commercial FEM software Abaqus. Since damage introduced stress and strain localizations, the robustness of the formulation is key to grant convergence, thus particular care was taken on the estimation of the Jacobian matrix ($d\sigma/d\varepsilon$). The formulation of the UMAT was made general (with independent modules) so that modifications of any module do not affect the global framework.

<Monitoring of void nucleation, subsequent growth, and coalescence during tensile tests>

To calibrate and validate the constitutive model, it is necessary to carry out specific experiment that keep track of the void distribution within the material and different strain level. In this regard, in situ tensile tests were conducted with carefully designed micro-tensile specimens, within an X-CT chamber available in our group. Tests was interrupted at regular strain levels and a complete scan of the region of interest was carried out by SEM on the surface and X-CT in the bulk to record the voids appearance and growth

４．研究成果

(1) To generate a multi-phase microstructure with controlled phase distribution, a new procedure was successfully developed. It is based on the binarization of the convolution product between a random field map sampled from a normal distribution and a multi-dimensional normal distribution. The parameters of the multi-dimensional distribution parameters may be estimated from experimental phase maps. Thereafter, the obtained phase map served as constraint to position elliptical seeds representing grains sampled from EBSD data. Finally, an anisotropic tessellation was applied to generate grain boundaries and attribute a crystal orientation based on the ODF and existing algorithm. The proposed method was successfully applied to Mg/LPSO and DP steels and reported in several publications.

(2) The phenomenological Hosford-Coulomb model, considering the effect of the equivalent plastic strain, stress triaxiality and Lode angle was successfully implemented in a CP model. It was found that strain localization caused by the softening of the stiffness matrix at damage initiation sites was responsible for a significant mesh size dependency due to a lower dissipated energy when mesh size decreased. To circumvent this drawback, a non-local averaging scheme was implemented to consider the weighted average fields around each integration point by introducing a single parameter gaussian weight function.

(3) The stress-strain paths of surface voids sites observed by SEM were estimated from CPFE simulation reproducing the same phase distribution as in the experiment. A new procedure was developed for the calibration of the damage initiation model based on the local stress-strain paths at void sites and their order of appearance. The procedure was tested on multiple DP steels with varying microstructures. The predicted damage initiation loci were found to be quite similar for the different materials which suggested that the damage mechanisms were similar and confirmed the robustness of the calibration procedure. In addition, the evolution of the void fraction and volume by X-CT with the strain and stress was used to calibrate the damage evolution post-initiation.

５．主な発表論文等

〔雑誌論文〕　計3件（うち査読付論文　3件／うち国際共著　3件／うちオープンアクセス　1件）

１．著者名 Briffod Fabien、Shiraiwa Takayuki、Enoki Manabu	４．巻 826
２．論文標題 Micromechanical investigation of the effect of the crystal orientation on the local deformation path and ductile void nucleation in dual-phase steels	５．発行年 2021年
３．雑誌名 Materials Science and Engineering: A	６．最初と最後の頁 141933～141933
掲載論文のDOI（デジタルオブジェクト識別子） 10.1016/j.msea.2021.141933	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Briffod Fabien、Hanqing Liu、Shiraiwa Takayuki、Enoki Manabu、Emura Satoshi	４．巻 892
２．論文標題 Crystallography and deformation behavior of α phase precipitate at twin/matrix interface in a cold rolled metastable Ti-12Mo alloy	５．発行年 2022年
３．雑誌名 Journal of Alloys and Compounds	６．最初と最後の頁 162234～162234
掲載論文のDOI（デジタルオブジェクト識別子） 10.1016/j.jallcom.2021.162234	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Briffod Fabien、Shiraiwa Takayuki、Enoki Manabu	４．巻 9
２．論文標題 The effect of the 18R-LPSO phase on the fatigue behavior of extruded Mg/LPSO two-phase alloy through a comparative experimental-numerical study	５．発行年 2021年
３．雑誌名 Journal of Magnesium and Alloys	６．最初と最後の頁 130～143
掲載論文のDOI（デジタルオブジェクト識別子） 10.1016/j.jma.2020.07.005	査読の有無 有
オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 該当する

〔学会発表〕　計7件（うち招待講演　0件／うち国際学会　1件）

１．発表者名 Briffod Fabien, Hu Haoyu, Shiraiwa Takayuki, Enoki Manabu
２．発表標題 Micromechanical investigation of stress-strain partitioning in dual-phase steel
３．学会等名 Japan Institute of Metals Lecture Meeting
４．発表年 2021年

１．発表者名 村山 恭平，加藤 翔也，Fabien Briffod， 白岩 隆行，榎 学
２．発表標題 X線CTによるDP鋼のボイド発展モデルの較正
３．学会等名 Japan Institute of Metals Lecture Meeting
４．発表年 2021年

１．発表者名 Fabien Briffod, Kyohei Murayama, Takayuki Shiraiwa, Manabu Enoki
２．発表標題 Micromechanical investigation of ductile void nucleation in dual-phase steels with varying
３．学会等名 The 7th International Conference on Advanced Steels（国際学会）
４．発表年 2021年

１．発表者名 Fabien Briffod, Takayuki Shiraiwa, Manabu Enoki
２．発表標題 Micromechanical behavior and crystal plasticity modeling of ductile void formation in a dual-phase steel
３．学会等名 Japan Institute of Metals Lecture Meeting
４．発表年 2021年

１．発表者名 加藤 翔也，Fabien Briffod ，白岩 隆行，榎 学，山崎 和彦
２．発表標題 DP鋼の組織最適化のための空間相関関数を用いた記述子選択
３．学会等名 Japan Institute of Metals Lecture Meeting
４．発表年 2021年

1．発表者名 村山 恭平，加藤 翔也，Fabien Briffod， 白岩 隆行，榎 学
2．発表標題 X線CTによるDP鋼のボイド挙動のモデルの検討
3．学会等名 Japan Institute of Metals Lecture Meeting
4．発表年 2021年

1．発表者名 白岩 隆行，加藤 翔也，Fabien Briffod，榎 学
2．発表標題 結晶塑性有限要素解析によるDP鋼の 組織-特性関係予測と逆問題解析
3．学会等名 The Iron and Steel Institute of Japan Lecture Meeting
4．発表年 2021年

〔図書〕　計0件

〔産業財産権〕

〔その他〕

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6．研究組織

	氏名 （ローマ字氏名） （研究者番号）	所属研究機関・部局・職 （機関番号）	備考

7．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

8．本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関