

Final Report for

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#1 Damage Evaluation for Ti Alloys in Creep based on Incompatibility Field Measurement via EBSD Technique

#2 Micro-Pillar Experiments Toward Identification of Roles of Dislocation Substructures on Fatigue Crack Initiation

Research Proposal to
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14. ABSTRACT

A definite limit of all the continuum models would be the inability of taking into account microscopic degrees of freedom in the constitutive framework. For crystalline metallic materials, microstructural degree of freedom in terms of dislocations is one of those sorts, which is currently recognized to be critically important to model and simulate multiscale aspects of deforming metals especially in plasticity. One and only sophisticated solution to this problem has been recently provided by the Field Theory of Multiscale Plasticity (FTMP) advocated by Hasebe (PI). In this new theoretical framework, such additional degrees of freedom are implemented via FTMP-based incompatibility tensor model, derived based on the differential geometrical curvature tensor for describing the metric defects of the crystalline space to be incorporated in a crystalline plasticity-based constitutive framework. This study aims at developing a new non-destructive damage evaluation technique based on field theory of multiscale plasticity (FTMP). Construction of an EBSD-based direct measurement technique of incompatibility tensor field is attempted by utilizing a data obtained under wedge indentation against a single crystal sample. Corresponding crystalline plasticity-based FE simulations are conducted with and without taking account of the FTMP-based incompatibility model. Major results obtained are presented in the report.

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Outline for #1a

A definite limit of all the continuum models would be the inability of taking into account microscopic degrees of freedom in the constitutive framework. For crystalline metallic materials, microstructural degree of freedom in terms of dislocations is one of those sorts, which is currently recognized to be critically important to model and simulate multiscale aspects of deforming metals especially in plasticity. One and only sophisticated solution to this problem has been recently provided by the Field Theory of Multiscale Plasticity (FTMP) advocated by Hasebe (PI). In this new theoretical framework, such additional degrees of freedom are implemented via FTMP-based incompatibility tensor model, derived based on the differential geometrical curvature tensor for describing the metric defects of the crystalline space to be incorporated in a crystalline plasticity-based constitutive framework.

This study aims at developing a new non-destructive damage evaluation technique based on field theory of multiscale plasticity (FTMP). Construction of an EBSD-based direct measurement technique of incompatibility tensor field is attempted by utilizing a data obtained under wedge indentation against a single crystal sample. Corresponding crystalline plasticity-based FE simulations are conducted with and without taking account of the FTMP-based incompatibility model. Major results obtained are presented in the following.

Results and Discussions for #1a

Here, an attempt is made to validate the FTMP-based incompatibility tensor model by reproducing a banded structure observed in the experimentally-evaluated geometrically-necessary (GN) dislocation density distribution under wedge indentation against a single crystal Cu sample reported by Kysar, et al.

Preliminary FEM analyses are firstly conducted to examine the appropriate boundary conditions for reproducing the experimental set-up. Banded structures similar to the experimentally-observed ones in the incompatibility distribution are demonstrated to emerge under the wedge indenter, affecting further the dislocation density distribution (equivalent to the GN distribution) to be correspondingly modulated (Fig.1a-1). Mesh size independency of the emerging bands is also confirmed, indicating one of the effectiveness of the present model. Some advanced analyses such as with extended dimensions of the simulation area are further conducted in a systematic manner (Fig.1a-2). The banded structures are shown to be formed in the relatively early stage of the indentation process, and the morphology is demonstrated to be basically maintained as the indentation proceeds. Comparisons with the experimental results are extensively made not only to validate but also to identify the deficiencies of the present FTMP-based model.

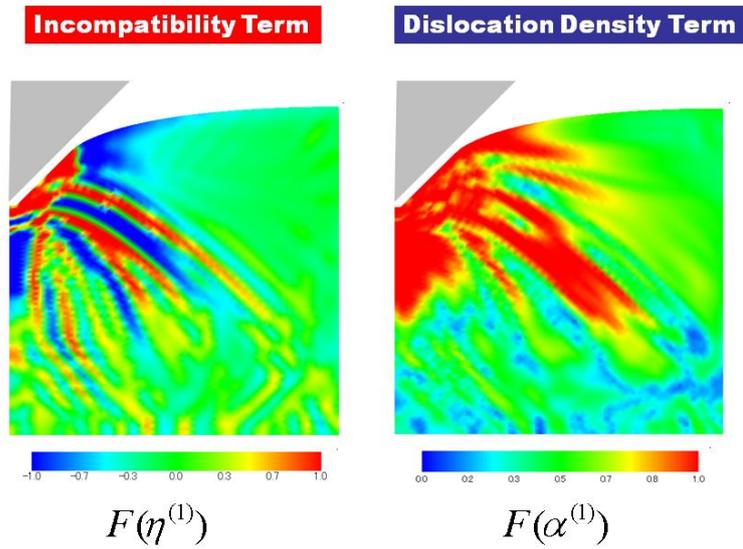


Fig.1a-1 Simulated deformation pattern emerged in FTMP-based incompatibility and dislocation density fields, qualitatively reproducing experimentally-observed GN distribution via EBSD technique

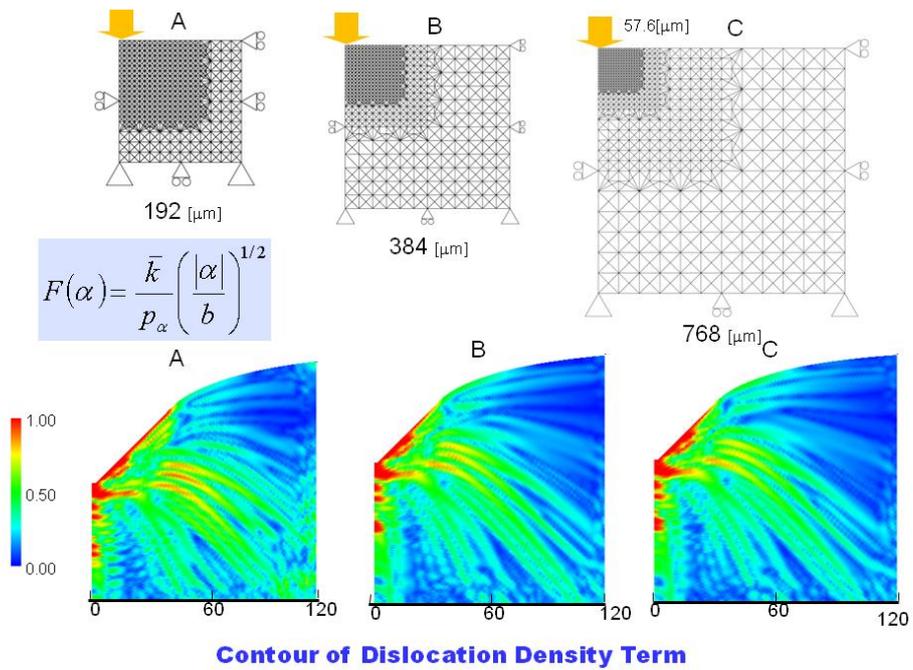


Fig.1a-2 Effect of model size and boundary condition on emerging banded structures under wedge indentation

Outline for #1b

This series of studies attempt to model and simulate the lath structures for high Cr steels under creep based on FTMP in conjunction with crystalline plasticity-based finite element analyses. FTMP-based incompatibility model is introduced in the microscopic constitutive equation to construct and ultimately simulate the evolution processes of the lath structure. Major conclusions derived in the study are summarized as follows.

Results and Discussions for #1b

(1)By applying tension to single crystal FEM models after introducing an initial strain distribution, we successfully reproduce the lath martensite block structure accompanied by fluctuating internal stress $\delta\sigma$ as well as the misorientation across the lath boundaries θ that crystallographically characterizes it. These additional factors, $\delta\sigma$ and θ , are employed afresh in the following creep analyses as initial conditions (Fig.1b-1).

(2)The effect of the additional factors on the creep behavior, e.g. minimum creep rate, is systematically examined. Both the factors are demonstrated to be critical for increasing the creep strength (decreasing creep rate), thus indispensable for modeling the martensite lath structures appropriately.

(3)Also revealed is a strong orientation dependency of the lath block on the creep strength, which has not been well-documented experimentally so far. The result implies an intrinsic inhomogeneity of the lath packet structures, which is the aggregates of randomly-oriented lath blocks, ultimately enhancing the inhomogeneous recovery.

(4)The lath block model constructed above is further applied to model lath packet structures with arbitrary morphology (Fig.1b-2). We extensively investigate the evolution of a packet structure made up of three lath blocks embedded within a single crystal matrix under creep. Critical importance of the additional factors, $\delta\sigma$ and θ , in appropriately modeling the enhanced creep properties are also confirmed. Moreover, an inhomogeneous recovery exclusively taken place near a boundary region of the consisting lath blocks is successfully simulated, which is further expected to be responsible for the accelerated deterioration of the creep strength of the targeted material.

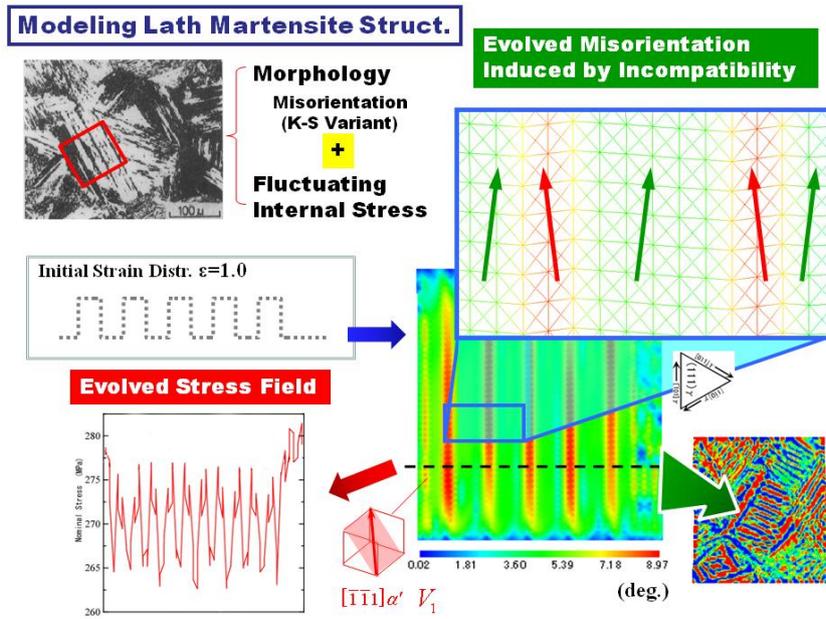


Fig.1b-1 Modeling of martensite lath block structure accompanied by fluctuating internal stress and misorientation based on FEM with FTMP-based incompatibility model

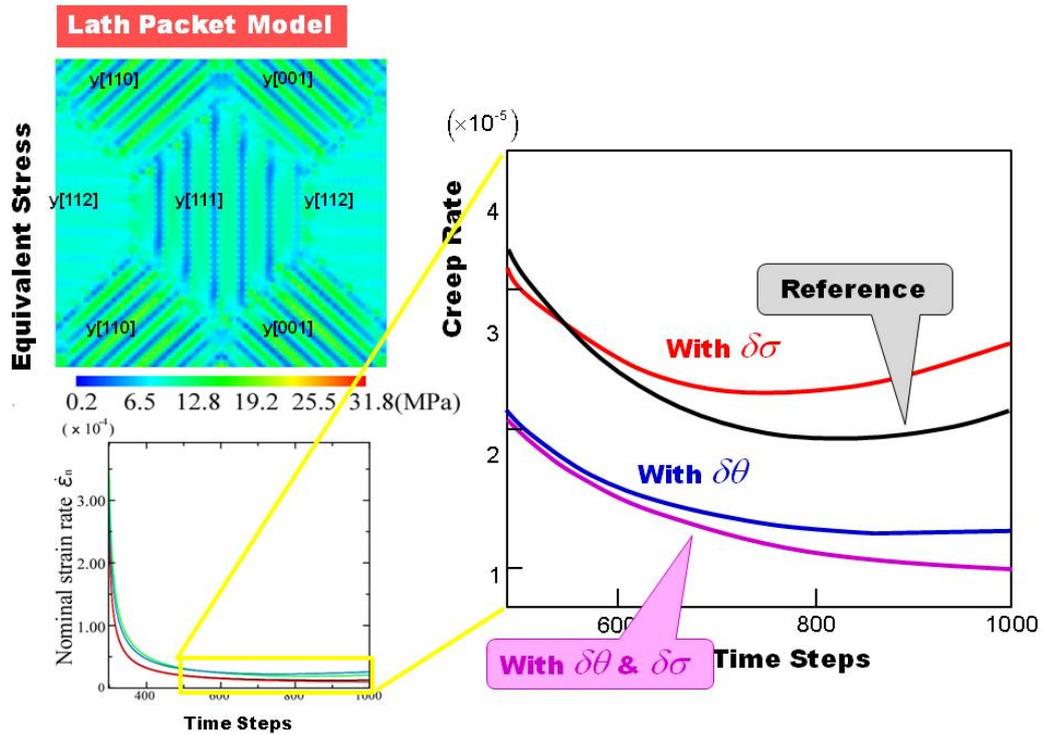


Fig.1b-2 Summary of FTMP-based simulation with a lath packet model for high Cr steel under creep, comparing the effect of fluctuating internal stress field and misorientation on creep strength.

Outline for #2

Myriads of experimental facts under a wide variety of loading conditions over a number of metals and alloys imply that a large fraction (70 to 80%) of the microscopic details of the nanoscale orders including those associated with individual dislocation motions and interactions with others are absorbed and stored at micrometer-order scale dislocation cell structures.

This series of studies examine first how the stored elastic energy of dislocation wall structures can vary depending on the arrangement of the wall-constructing dislocations, by assuming representative three wall structures of dislocations with constant density.

Secondly, modeling and simulation of a transient process from a slip band to a fatigue crack based on FTMP is attempted. FTMP-based incompatibility model is introduced to a constitutive equation within the framework of crystalline plasticity, and cyclic straining analyses are conducted on a single-slip oriented Cu single crystal model by using FEM. Reproduction of a slip band with a PSB-ladder-like internal structure is attempted assuming initial conditions with and without corresponding strain distributions. After discussing the slip concentration, cyclic stress response, stored elastic strain energy, accumulated plastic work and its dissipation into heat at the PSB region, the present study extensively examined possible transition mechanisms toward the growth of grooves thereabout and that into crack. Major results obtained are summarized as follows.

Results and Discussion for #2

(1) Elastic strain energy stored in the wall structures are calculated and comparison is made among the three arrangements (Fig.2-1). Dipolar wall (extreme left) shows smallest value due to effectively-screed stress field of both-signed dislocations, whereas the cell wall model (extreme right) exhibits the largest among the three. To be emphasized is there extended over three order magnitude of difference in the stored elastic strain energy depending on the wall-constructing dislocation arrangements even with the same dislocation density.

(2) A slip band-like region having a substructure mimicking PSB ladder is demonstrated to be spontaneously formed across the single crystal sample rather promptly under plastic strain amplitude-controlled cyclic loading (Fig.2-2), provided the FTMP-based incompatibility model is active as well as the cyclic straining axis coincides with the single slip orientation.

(3) Activation of the FTMP-based incompatibility model in the constitutive equation (hardening law) is shown to be crucial not only for generating the ladder-like substructure but also for promoting salient strain concentration at the banded region: The inactivation of it results in (A) a similar slip concentration but with no appropriate substructure, and (B) no significant strain concentration there. Also

demonstrated is the strain concentration is accompanied by the evolving tensile mean stress, which is expected to promote mode I-type crack initiation and further extension (Fig.2-3).

(4)A preliminary simulation for the transition process from PSB to a surface crack is attempted. Based on a “flow-evolutionary” working hypothesis, the FTMP-based incompatibility term for the vacancy field, assumed to be produced from interactions of dislocations in the PSB ladder region, is artificially introduced in the hardening law. The sample surface near the edge of the band with the vacancy-induced incompatibility term demonstrated to be receded, implying a growth of a groove to be ultimately evolved into a crack under successive straining cycles.

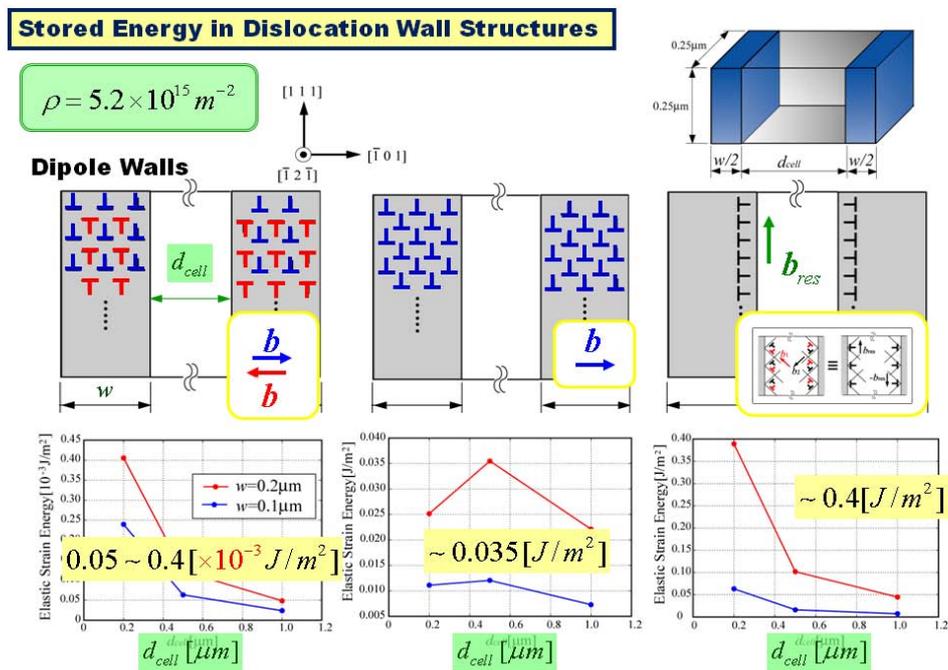


Fig.2-1 Summary of the calculated elastic strain energy stored in the wall structures comparing the three arrangements.

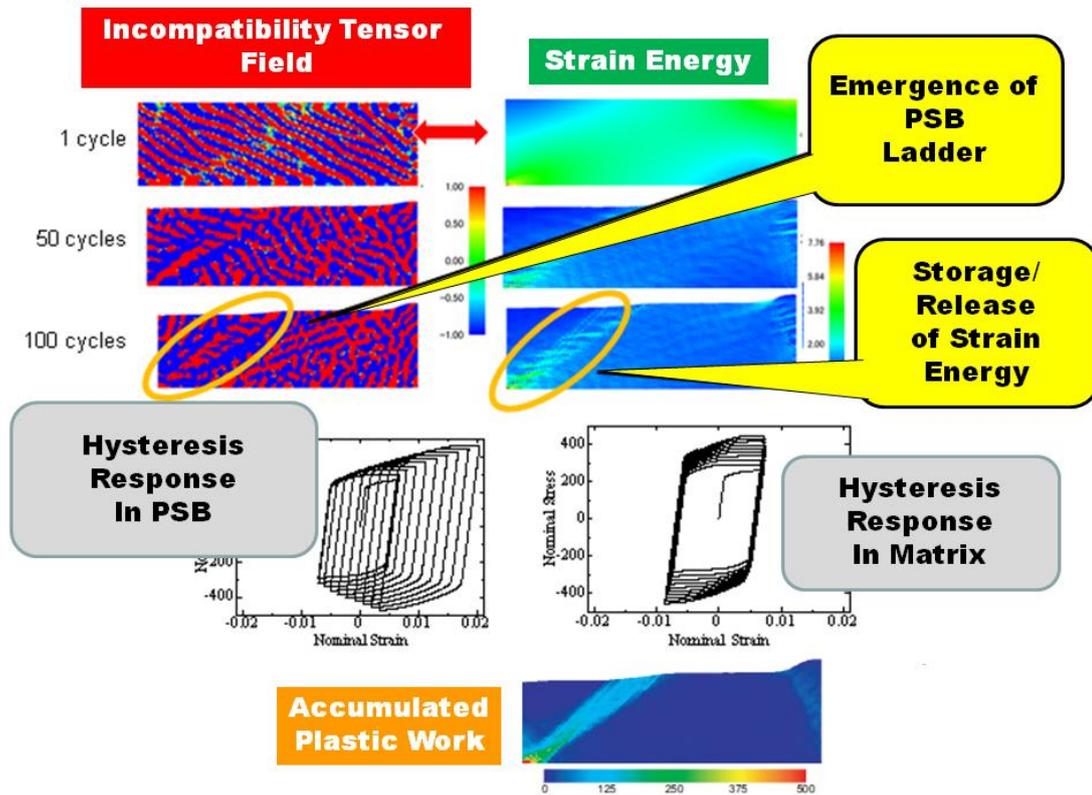


Fig.2-2 Spontaneously-evolving PSB with ladder-like substructure within vein-like matrix under cyclic straining, together with corresponding elastic strain energy and plastic work exclusively accumulated in banded region .

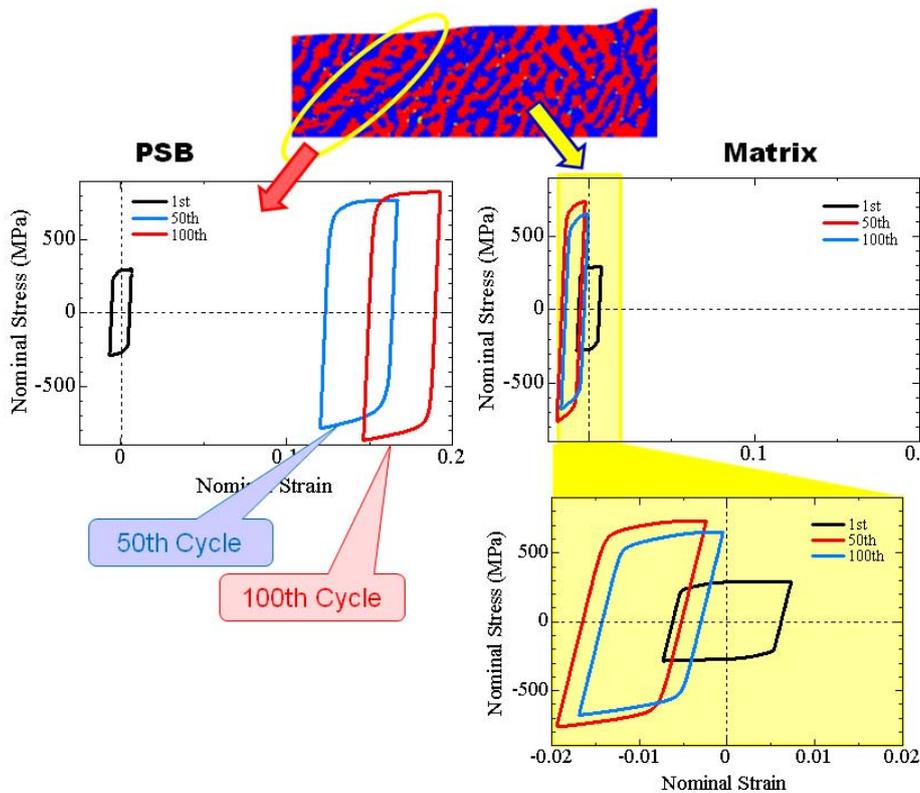


Fig.2-3 Hysteresis response of banded region exhibiting not only strain concentration but also evolving mean tensile stress.

References

Kysar, J.W., Gan, Y.X., Morse, T.L., Chen, X. and Jones, M.E., (2007), “High Strain Gradient Plasticity Associated with Wedge Indentation into Face- centered Cubic Single Crystals: Geometrically Necessary Dislocation Densities,” *J. Mech. Phys. Solids*, **55** (7), 1554–1573.