

Final Report for

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**"Multiscale Computational Design Optimization of
Copper-Strengthened Steel for High
Cycle Fatigue"**

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14. ABSTRACT Abstract: This research project performed FTMP-based modeling of surface groove formations that ultimately evolve into a crack and the effects of dislocation substructures were considered. Cu-added steels were studied as a model system. As definitive steps toward it, roughly three sub-divided subjects are dealt with: They are (1) effects of Cu addition on the core structure of a screw dislocation in Fe, approached through ab initio-based calculations, (2) Field-theoretical evaluations of dislocation cell structures in terms of flow-evolutionary law (i.e., fluctuations in incompatibility tensor field versus elastic strain energy) and (3) modeling of a slip band (of PSB ladder underlying structure) and attendant crack initiation process.					
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Outline

This research project aims at a FTMP-based modeling of surface groove formations to be evolved ultimately into crack, considering the effect of the underlying dislocation substructures (ultimately for Cu-added steels). As definitive steps toward it, roughly three sub-divided subjects are dealt with: They are

- (A) Effects of Cu addition on the core structure of a screw dislocation in α -Fe, via *ab initio*-based calculations.
- (B) Field-theoretical evaluations of dislocation cell structures in terms of flow-evolutionary law (i.e., fluctuations in incompatibility tensor field versus elastic strain energy).
- (C) A modeling of a slip band (of PSB ladder underlying structure) and attendant crack initiation process.

Major results obtained are presented in the following.

Results and Discussions for (A)

Figure 1 summarizes the output obtained for (A), where screw dislocation cores for α -Fe with and without Cu rows are compared. Transition of the structure from non-polarized to fully-polarized, together with changes in the Peierls stress, is demonstrated to take place with the addition of Cu. Also revealed is a meta-stable configuration of the screw core under external shear stress. For details, please refer to [Chen, et al. (2007)].

Results and Discussion for (B)

In this category, by utilizing 2D and 3D simulation results for dislocation cell structures based on field theory, the associated incompatibility fields and elastic strain energy distributions are evaluated, ultimately to obtain the duality coefficient κ in the flow-evolutionary law, i.e., $\eta_{ij} = \kappa \delta T_{ij}$ (η_{ij} : incompatibility tensor, $\delta T_{ij} \equiv T_{ij} - \langle T_{ij} \rangle$: energy-momentum tensor). Figure 2 compares the obtained κ between those based on correlation functions $\langle \delta \eta_{ij} \delta \eta'_{ij} \rangle$ and $\langle \delta T_{44} \delta T'_{44} \rangle$. Smaller κ in well-developed cells implies that the dislocation cell structures tend to yield (1) larger amount of excessively-stored strain energy, (2) larger Bauschinger effect (especially transient softening), and (3) larger surface roughness to be evolved during plastic deformation, which differentiate the morphology from others, e.g., vein and planar structures of dislocations.

Results and Discussion for (C)

(C-1) Modeling PSB

For modeling a persistent slip band (PSB), FTMP-based incompatibility tensor field model is used to mimic the banded region, simply by introducing initial strain distributions. Figure 1 displays a summary of the results, showing an example of the reproduced PSB under $\Delta\gamma^p$ -controlled cyclic deformation, where the contour of the incompatibility term $F(\eta^{(\alpha)})$ and the corresponding strain distribution are presented. Relatively concentrated shear plastic deformation in the band region,

especially in the channels is shown to be successfully reproduced. We also confirm two things; (i) increasing strain energy approaching the surface, and (ii) alternating high and low strain energy corresponding to the ladder wall and channel regions, respectively. These trends turn out ultimately to be desirable for both the vacancy concentration and the diffusion toward the surface (see below (C-2)).

(C-2)Surface Groove Formation

For simulating crack initiation processes at the sample surface, we need at least one more factor, e.g., dislocation-induced vacancy formation and their diffusion, without which material dependencies cannot be explicitly taken into account. This study thus separately makes an attempt to simulate the vacancy diffusion processes toward the surface along the band, in conjunction with the results in (C-1). A diffusion equation proposed by Ortiz, et al. [Repetto and Ortiz (1997)] is tentatively used, which includes enhanced diffusion depending on the gradient of strain energy.

Figure 4 shows a model used in the simulation, assuming several distributions of strain energy W along the PSB. Here, the most suitable W distribution (Pattern-A) and the associated vacancy flux distribution at the surface are displayed. From thus obtained variation of vacancy flux distribution with time, we can virtually simulate changes in the surface profile. The corresponding velocity for the surface to recede is evaluated as,

$$v_n^{surface} = \mathbf{j}_{vacancy} \cdot \mathbf{n}_{surface}$$

Four cases are assumed in terms of the relative position of the wall against the surface. Since the vacancy flow will be sensitively affected by the condition, it is expected to control the groove formation behavior. The simulation results are displayed in Fig.5, where the resultant surface grooves under 4 conditions are compared. As demonstrated, the wall position has dominant effect on the vacancy flow-driven groove formation. With the given strain energy distribution, the grooves are basically formed at the band edges, except Case (a), in which the wall is facing the surface. The closer the wall is located from the surface, the faster the surface recedes. Cases (b) and (d) seem to be equivalent but they will be differentiated when additional gradient in the strain energy is superimposed, as will be discussed further.

Note, there are plural dislocation processes taken place within both the wall and channel regions. This approach focuses on those in-between the channels, especially interactions among mutually-passing and interacting screw segments under to-and-fro motion, eventually producing vacancies as a product of dipole annihilation. Such interaction can be taken place either at the wall and the channel regions, supposed to produce a vacancy. The processes have been confirmed based on dislocation dynamics simulations [El-Awady (2008), Erel (2009)].

Conclusion

In this project, we clarified the following based on FTMP-based modeling and simulations; (A)transition of the screw dislocation core structure of α -Fe via additions of Cu precipitates, (B)potential roles of dislocation substructures (cells) for surface roughening, and (C)decisive roles of PSB walls for surface crack initiation.

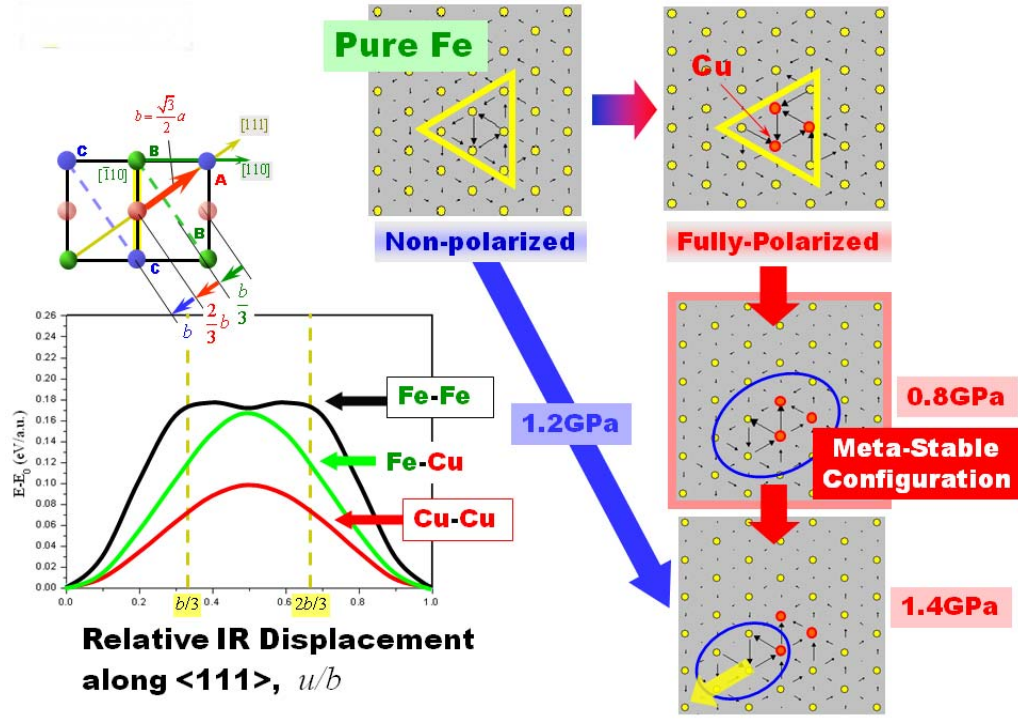
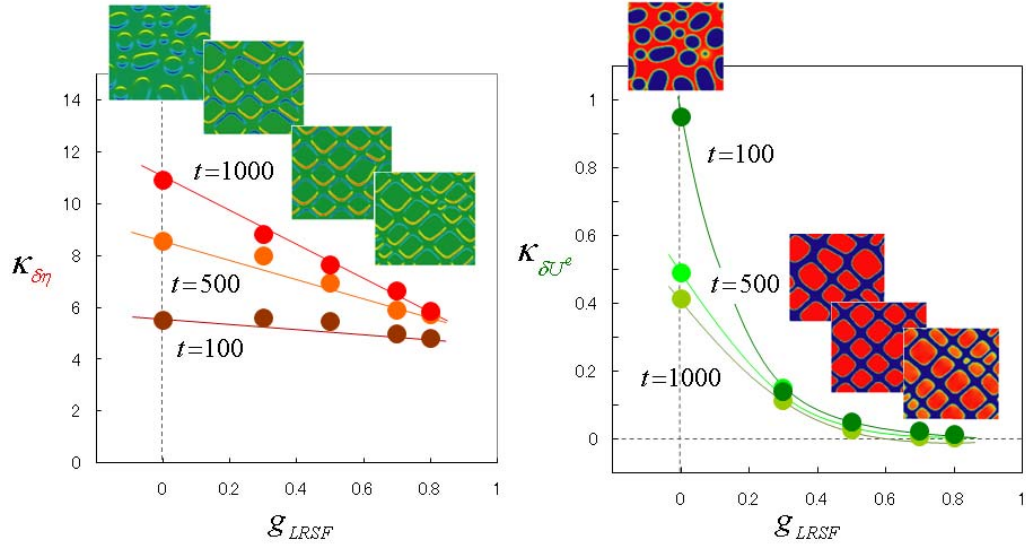


Fig.1 Summary of *ab initio*-based calculation for a screw dislocation core of α -Fe with and without Cu clusters.



$$\kappa_{\delta\eta} = \frac{1}{\Omega} \int_{\Omega} \langle \delta\eta(x) \delta\eta(x') \rangle d\Omega \quad \kappa_{\delta U^e}^{-1} = \frac{1}{\Omega} \int_{\Omega} \langle \delta U^e(x) \delta U^e(x') \rangle d\Omega$$

$$\Rightarrow \kappa_{\delta\eta} = \|\delta\eta\| \cdot \xi_{\delta\eta} \quad \Rightarrow \kappa_{\delta U^e}^{-1} = \|\delta U^e\| \cdot \xi_{\delta U^e}$$

$$\quad \quad \quad \equiv 1$$

Fig.2 FTMP-based evaluation of duality coefficient k in flow-evolutionary law for dislocation cell structures, comparing those via incompatibility field and elastic strain energy fluctuation.

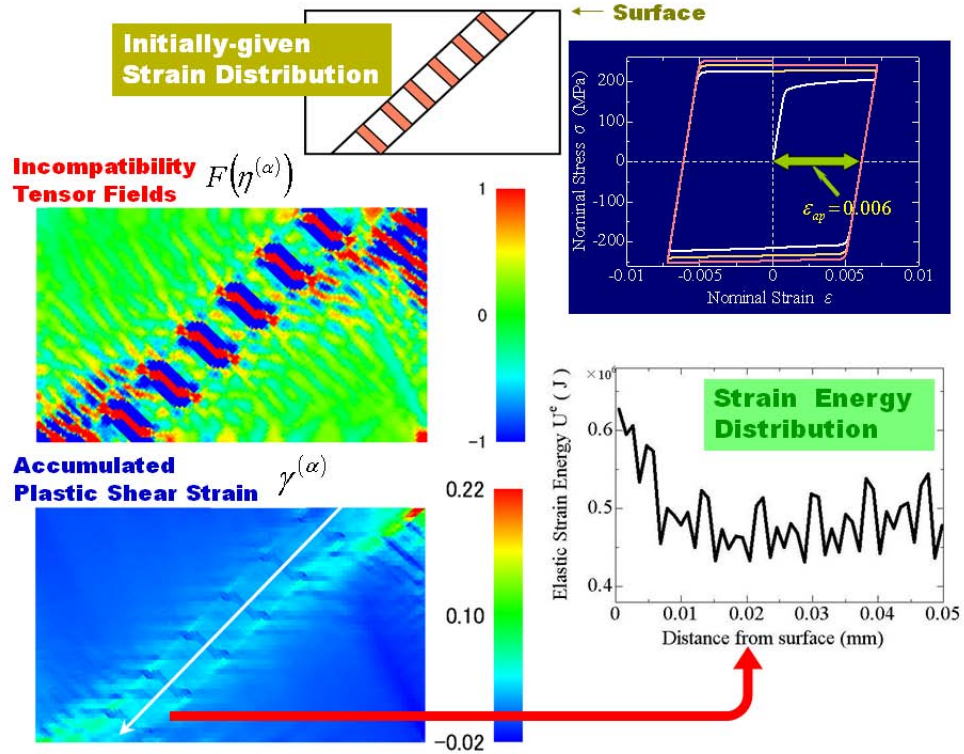


Fig.3 FTMP-based PSB model developed under cyclic straining, together with contours of incompatibility field, plastic shear strain and distribution of strain energy along PSB.

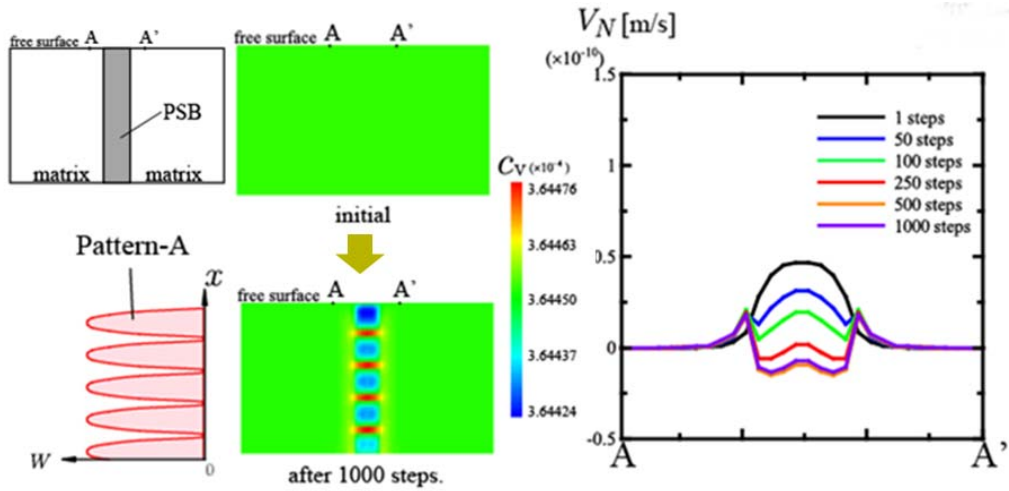


Fig.4 Computational model for vacancy diffusion analysis, initially assuming strain energy distribution along PSB. Right shows variation of vacancy flux at free surface.

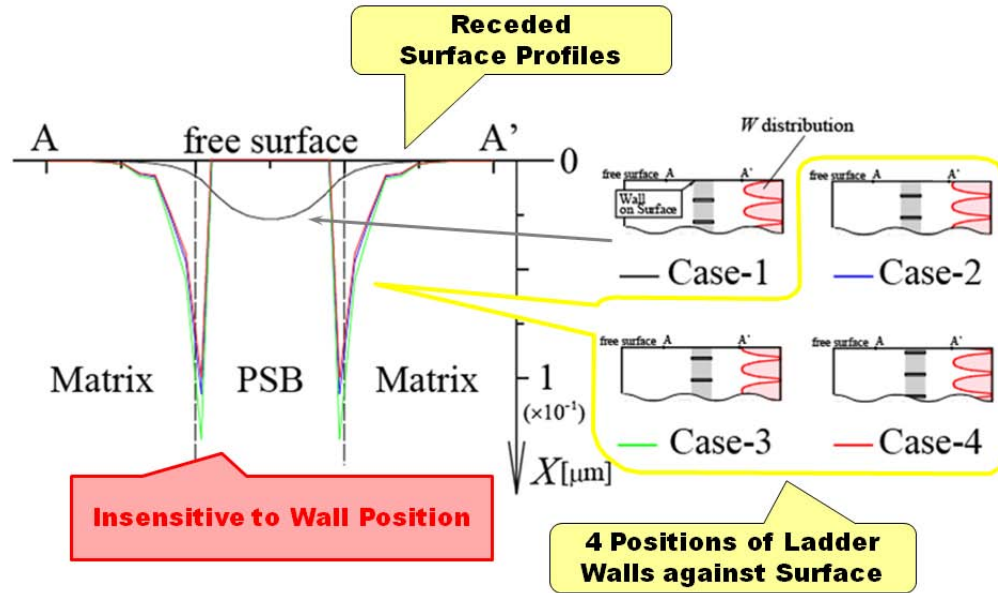


Fig.5 Comparison of simulated surface grooves after 1000 steps among four wall positions against free surface, demonstrating case insensitive nature of the process.

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