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Field Theoretical Multiscale Polycrystal Plasticity

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This paper clarifies the essential features of polycrystalline plasticity resulting from collective behavior of large number of composing grains. Hydrostatic stress and deviatoric strain fluctuations become large with increasing number of grains and they can be a key for polycrystal plasticity modeling. Applicability of the present viewpoint to dual phase materials with hard phase is extensively discussed.
Key words: Polycrystal, Crystal Plasticity, Field Theory, Field Fluctuation

1. INTRODUCTION

Multi-scale modeling has been becoming a key word for the substantial bridge between microscopic phenomena and macroscopic behavior of materials transcending over hierarchical structures. Highly progressed computer ability as well as sophisticated computational techniques has promoted such trend. Until quite recently, discussions on "polycrystals" have been rather concentrated on how to realistically evaluate the averaged stress-strain response, focusing on relaxed constraint even with FEM simulations. On the other hand, deficiencies of "oligo grain" models containing much-smaller-number-grains than reality has been repeatedly pointed out in simulating polycrystal behavior based on FEM, however, no one have pointed out what really the "deficiencies" are.

The author [1] has recently proposed a new perspective dictating that fluctuations of the grain-wise stress and strain fields can be an essential feature of polycrystalline plasticity.

This paper discusses theory and modeling for polycrystalline materials including nano-crystals based on the field theory of plasticity advocated recently by the author [2, 3]. Emphasis here is placed on the collective effect of a large number of composing grains on meso- and macroscopic deformation behavior of polycrystals. For this purpose, a series of systematically designed finite element simulations have been conducted.

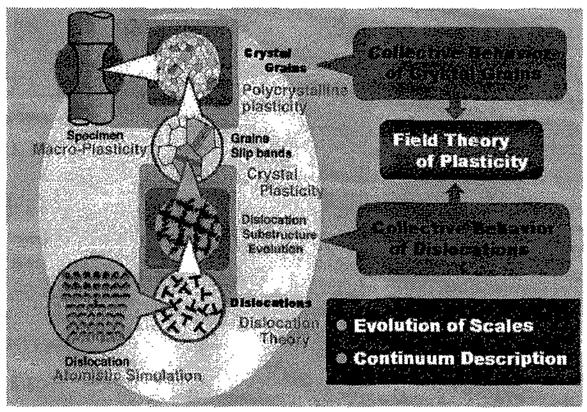


Fig. 1 Hierarchy of polycrystal plasticity and key scales for multi-scale modeling.

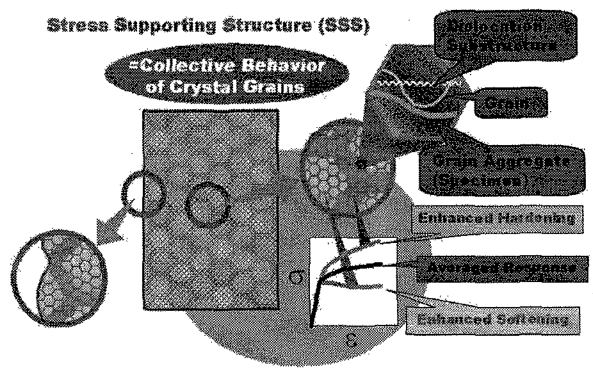


Fig. 2 Schematics of mesoscopic structure as a result of collective behavior of crystal grains, together with "role sharing" of grains.

2. FIELD THEORY OF PLASTICITY

Figure 1 illustrates hierarchical structure of polycrystal plasticity emphasizing two key hierarchies, both relating to "collective effects" of entities, i.e., dislocations and crystal grains. The former leads to substructure evolution and has been dealt with in the other paper [2]. The latter has not been well documented so far and will be discussed in the present paper. Figure 2 shows hypothetical schematics of the collective effects of grains, i.e., trans-granular mesoscopic stress supporting structure (SSS). One of the manifestations would be, for example, the surface roughness of the order of the wavelength of SSS during plastic deformation.

In order to capture the essence of the multiscale plasticity-related phenomena, at least three scales of inhomogeneities have to be considered. They are (a)dislocation substructure (b)crystal grain and (c)aggregate of grains, e.g., SSS described above. Particularly, the scales (a) and (c) attribute to more or less the collective behavior of the composing elements, i.e., dislocations for (a) and crystal grains for (c). There, qualitatively new characteristic scales spontaneously emerge and they essentially control the upper scale phenomena. The scale (b), on the other hand, affects both

(a) and (c), and, at the same time, is affected back them. Practically the level (b) has been used in controlling mechanical properties by alloying and introducing metallurgical structures.

3. MODEL DESCRIPTION

To identify key factors of modeling polycrystalline aggregate, especially the collective effect of a large number of composing grains on the mesoscopic deformation behavior including the SSS formation, systematically designed finite element (FE) simulations are made.

Figure 3 shows finite element polycrystalline models used in the present study. The models have a common representative area, containing 23 grains with a same orientation distribution surrounded by different numbers of grains. The total numbers of grains are 23, 77, 168, 613, 1073 and 1661. All the grains here are assumed to have the same hexagonal shape to eliminate additional factors, e.g., size distribution and morphology, other than the "number" effect. Each grain is divided into 576 to 64 triangular elements as listed in the inserted table in Fig.4. Plane strain two slip system is assumed here to introduce the highest constraint to the grain deformation. Constitutive equation and related models employed in the analysis are listed in Fig.5.

Boundary conditions for the present analysis are illustrated in Fig.4. Tension up to 30% nominal strain is applied with laterally traction free condition. In what follows, grain-wise stress-strain responses will be mainly discussed, where averages of stress and strain are taken over each grain, in order to focus on the effect of collective behavior of grains.

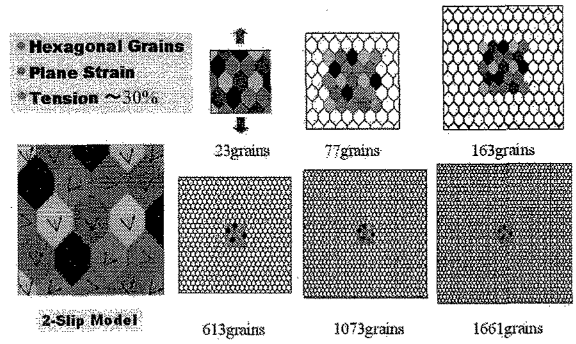
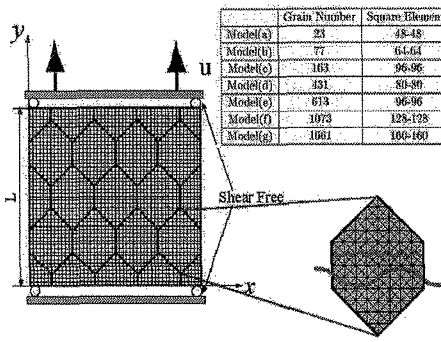


Fig. 3 Polycrystalline models used in FE analysis. Each grain is divided into several hundred to several ten meshes.



	Grain Number	Square Elements	Triangle Elements
Model(a)	23	48-48	576
Model(b)	77	64-64	256
Model(c)	163	96-96	256
Model(d)	431	80-80	64
Model(e)	613	96-96	64
Model(f)	1073	128-128	64
Model(g)	1661	160-160	64

Fig. 4 Boundary condition of present analysis together with mesh division of each grain.

Constitutive Model

Constitutive Equation (Peirce, D., et al, 1983)

$$\overset{\nabla}{S}_{ij} = C^{e}_{ijkl} : d_{kl} - \sum_{(\alpha)} R^{(\alpha)}_{ij} \dot{\gamma}^{(\alpha)}$$

Microscopic Constitutive Relation (Hutchinson, J. W., 1976)

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}^{(\alpha)}_{ref} sgn(\tau^{(\alpha)}) \left(\frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right)^{\frac{1}{m}}$$

Referential RSS (Ohashi, T., 1987)

$$g^{(\alpha)} = \tau^{(\alpha)}_{y} + \sum_{\beta} \mu \tilde{b} a \Omega_{\alpha\beta} (\rho^{(\beta)}_{a})^{\frac{1}{2}}$$

Hardening Coefficient

$$h_{ab} = \frac{\Omega_{ab}\, a\, \mu\, \tilde{b}}{2\sqrt{\rho^{(b)}_{a}}} \left(\frac{1}{L^{(b)}} - 2\, y_c\, \rho^{(b)}_{a} \right)$$

Fig. 5 Constitutive models used in present study.

4. RESULTS AND DISCUSSION

4.1 Single Phase Models

Figure 6 summarizes the obtained results where grain-wise stress-strain curves are shown. Growing fluctuations in stress and strain fields, $\delta\sigma$ and $\delta\varepsilon$, with increasing number of grains are observed while the macroscopic stress-strain curve stays unchanged. The results imply that the field fluctuations are the natural consequence of the collective behavior of the composing grains because morphological effects are eliminated in the present model. Therefore, the existence of the stress and strain fluctuations is considered to be an essential feature of the polycrystalline plasticity. Note that, as far as the macroscopic response is concerned, the fluctuations do not always have to be considered because they are macroscopically "invisible" being averaged out.

Further decompositions into deviatoric and hydrostatic components can clarify the roles of the above field fluctuations, i.e.,

$$\delta\sigma = \delta(\sigma' + \sigma_m I) = \delta\sigma' + I\delta\sigma_m$$

$$\delta\varepsilon = \delta(\varepsilon' + \varepsilon_v I) = \delta\varepsilon' + I\delta\varepsilon_v$$

The inserts in Fig. 6 show schematics of obtained results for the corresponding correlations. There observes small fluctuation in the deviatoric stress whereas relatively large fluctuation exists in the deviatoric strain component.

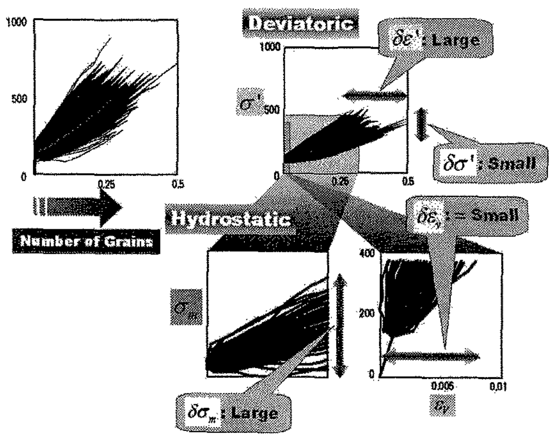


Fig. 6 Summary of simulation results demonstrating clear collective effects of increasing number of grains on stress-strain response of polycrystalline aggregate.

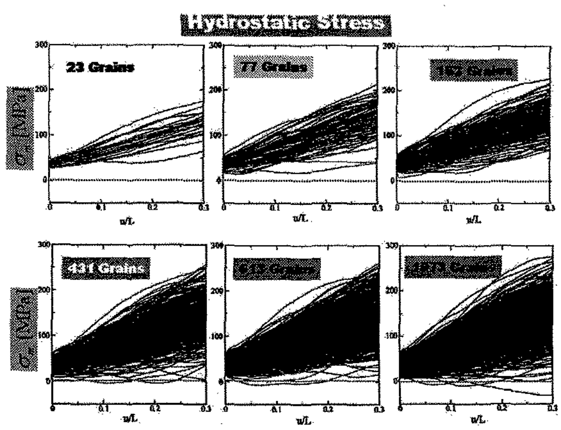


Fig. 7 Examples of simulation results showing growing fluctuation of hydrostatic stress with increasing number of composing grains.

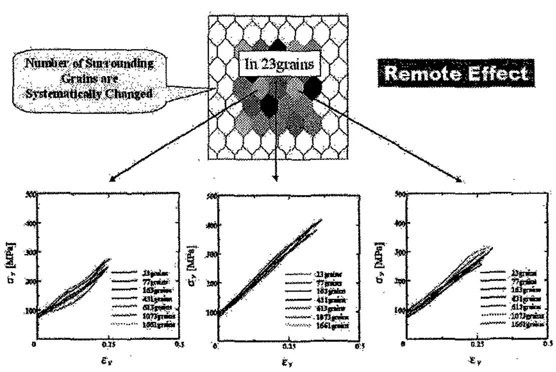


Fig. 8 Stress-strain responses of representative grains affected by number of surrounding grains implying "remote effect."

On the other hand, quite large fluctuation in the hydrostatic stress is demonstrated to exist. Therefore, the origin of the stress fluctuations is concluded to be attributed to the hydrostatic components. The fluctuation of the volumetric strain is elastically proportional to that of the hydrostatic stress, however, the magnitude is negligibly small comparing with total strain range. Figure 7 shows the results for the hydrostatic stress plotted against nominal strain. One can see the growing fluctuations as the number of grains increases.

Figure 8 shows variation of stress-strain response of several grains in the representative area with number of surrounding grains. It is shown that the stress-strain curves are more or less influenced by the grains in the surroundings even with the same combination of neighboring grains in the common area. Also confirmed is the same trend when the randomness of the orientation in the surrounding grains is changed. These results clearly imply that the stress response of a grain is not determined only by its immediate neighbors but is greatly affected by the grains in the distances, meaning that there exists a "remote effect" activated through the SSS. The "remote effect" caused by the collective effect of large number of grains makes difficult to identify the "representative volume" with periodic boundary conditions.

Further rearrangements of the above results with

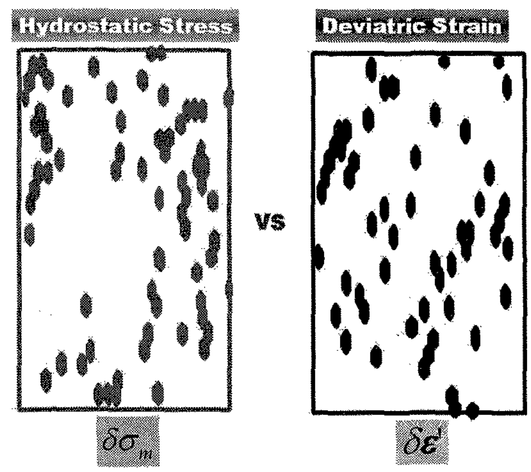


Fig. 9 Comparison of hydrostatic stress and deviatoric strain distributions implying "role sharing" between the two.

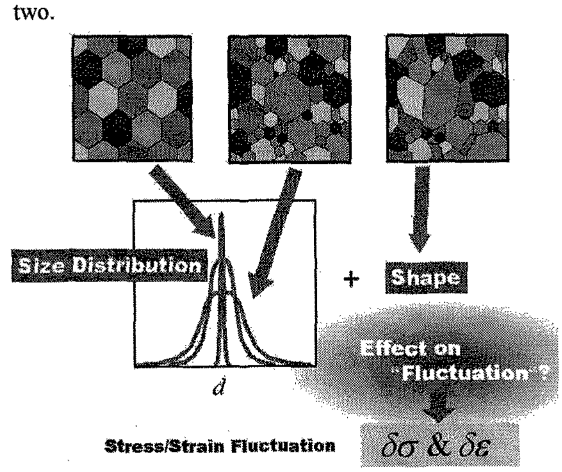


Fig. 10 Schematic illustration for distributed grain size models.

respect to the hydrostatic and deviatoric components reveal that the "remote effect" is mainly due to the hydrostatic stress and deviatoric strain components. Note that any coarse-grain models fail to capture these important aspects of polycrystalline behavior.

Figure 9 displays distributions of hydrostatic stress and deviatoric strain, where only grains having values above certain thresholds are shown for simplicity. The structure evolution like SSS is not obvious at this stage probably because of the relatively small number of grains in the present model.

Comparison of the two distributions indicates that they do not generally coincide. This may be regarded as a sort of "role sharing" between stress support and deformation transmission, which will be another essential feature of the polycrystalline plasticity. Details of this "role sharing" including its actual "role" in determining the overall deformation behavior will be discussed in the coming paper.

From the above discussions, it is tentatively concluded that the stress fluctuation mainly arises from that of the hydrostatic component $\delta\sigma_m$, while the strain fluctuation attributes to the deviatoric component $\delta\varepsilon'$. Since the morphological effects are basically eliminated here, these field fluctuations are natural, peculiar to polycrystalline aggregates. Introducing grain size distributions is demonstrated to yield basically the same trend.

4.2 Distributed-Grain Size Models

One of the strong advantages of the present viewpoint based on the field fluctuations is the applicability to more complex and practical situations. Figure 10 is a schematics of the models with distributed grain size which is expected to affect $\delta\sigma_m$ and $\delta\varepsilon'$. Tentative simulations support this although the details are not shown here because of the page limitation.

4.3 Dual Phase Models

Dual phase model where hard grains are introduced is also examined to see the effect of artificially introduced heterogeneities on the field fluctuations. Here the flow stress level ten times larger than the matrix grain is assumed and the discussion is limited to 25% volume fraction with 613 grains as illustrated in Fig.11. As shown in the figure, two types of hard phase distribution are considered, i.e., uniform (Model 1) and non-uniform (Model 2).

Figure 12 schematically displays the obtained results comparing with those for the single phase model discussed above. The dual phase models exhibit even larger field fluctuations, i.e., $\delta\sigma_m$ and $\delta\varepsilon'$, than the single phase model, whereas there observed also small fluctuation in the deviatoric stress components. Particularly, $\delta\sigma_m$ becomes more than double.

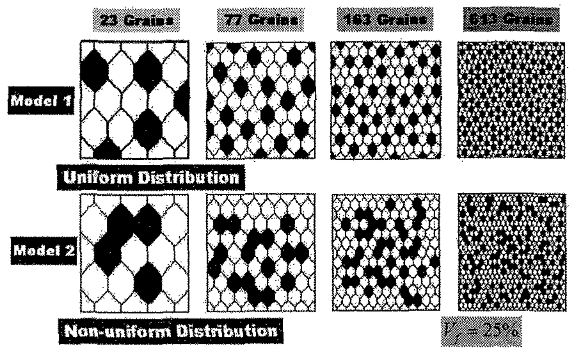


Fig. 11 Dual phase models used where hard grains having larger flow stress level are introduced with 25% volume fraction.

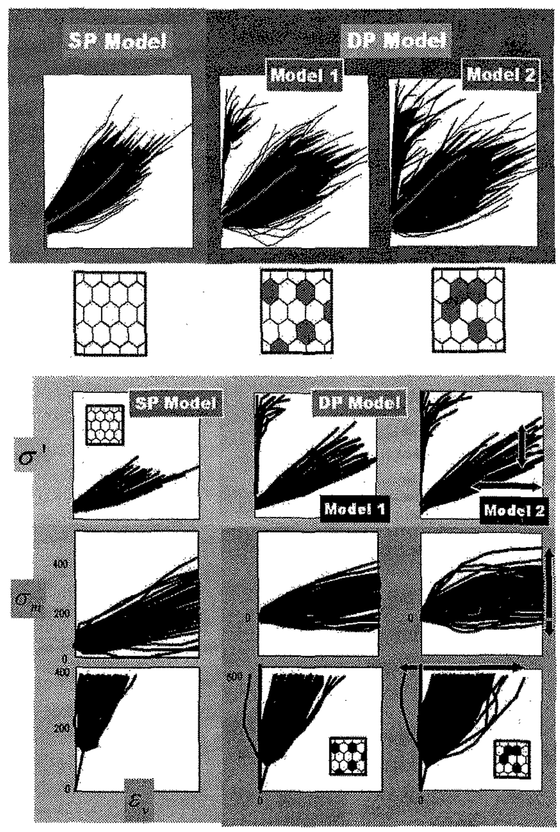
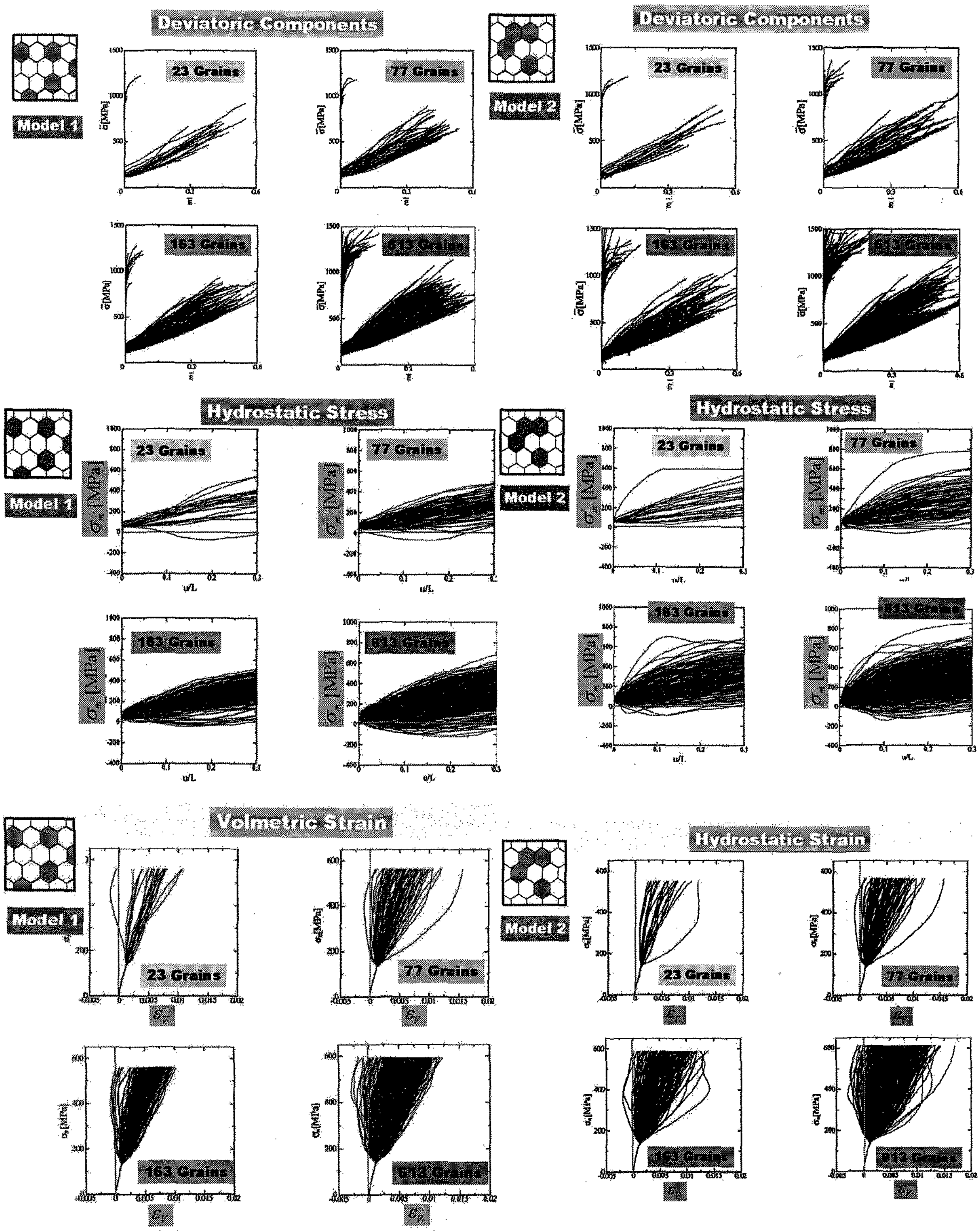


Fig. 12 Schematics of simulation results for dual phase models comparing with those for single phase model.

Accordingly volumetric component of strain $\delta\varepsilon_v$ becomes non-negligibly large in this case. This larger $\delta\varepsilon_v$ may be one of the key features in modeling dual-phase polycrystals because it will affect, e.g., void nucleation and growth behavior controlling ductile fracture.

It is also shown that introducing non-uniformity in the hard phase distribution can greatly change the field fluctuations. Model 2 exhibits even larger fluctuation of the hydrostatic stress as well as deviatoric strain than Model 1.



(a) Model 1 (uniform distribution) (b) Model 2 (non-uniform distribution)

Fig. 13 Examples of simulation results showing fluctuations of stress and strain components with increasing number of composing grains for dual phase models with (a)uniform and (b)non-uniform distributions of hard phase.

Figure 13 shows individual results for both the models demonstrating increasing fluctuations of hydrostatic stress as well as small fluctuations of deviatoric stress.

4.4 Examples of Applications

Lüders banding is well-known to become significant for finer-grain well-annealed mild steels. Finer grains mean inclusion of larger number of grains, so that this case would yield larger $\delta\sigma_m$ even before yielding with fine SSS. Enhancement of $\delta\varepsilon'$, which is the dual of $\delta\sigma_m$, is restricted owing to the large critical resolved shear stress (CRSS) common to low-carbon steels based on pinning by carbon solutions. Once the unpinning occurs at a certain place of a specimen, it triggers the avalanche of $\delta\varepsilon'$ across the specimen. The width of the band will coincide with the wavelength of the SSS. This is the Lüders band and is propagated throughout the specimen with a speed controlled by the energy-momentum tensor. Note the large CRSS resulted from low mobility of the screw dislocation originated from its complex core structure.

Examples of extremely large number of crystal grains are ultra fine grained (UFG) and nano-crystalline materials which are basically the same as the above case as schematically illustrated in Fig.14. This case is expected to yield clearer role-sharing between $\delta\sigma_m$ and $\delta\varepsilon'$. Large $\delta\sigma_m$ tends to go to grain interiors because of the large long-range stress field. Consequently $\delta\varepsilon'$ will concentrate on grain boundaries and it will drive grain boundary sliding. The long-range stress field within grains is considered to be originated from the so-called "non-equilibrium" grain boundary, which needs separate discussion.

5. CONCLUSIONS

This paper provided the first substantial approach toward modeling "polycrystalline" plasticity beyond the "averaged" behavior, and clarified the deficiencies of the conventionally-used "coarse-grain" or "oligo-grain" models in simulating general features of polycrystalline aggregates in the following respects.

(1)Stress and strain fields greatly fluctuate as the number of grains increases. Stress fluctuation is mainly attributed to the hydrostatic components whereas strain fluctuation is due to that of deviatoric component.

(2)Stress-strain response of a grain is not determined by the information of its immediate neighbors but is greatly affected by the remote grains implying "remote effect."

(3)The "remote effect" caused by the collective effect of large number of grains makes difficult to identify the "representative volume" with periodic boundary conditions.

(4)Applicability of the present scope based on the field fluctuations are briefly examined by taking well-known examples, i.e. Lüders banding and grain boundary sliding in ultra fine grained (UFG) and nano-crystalline materials.

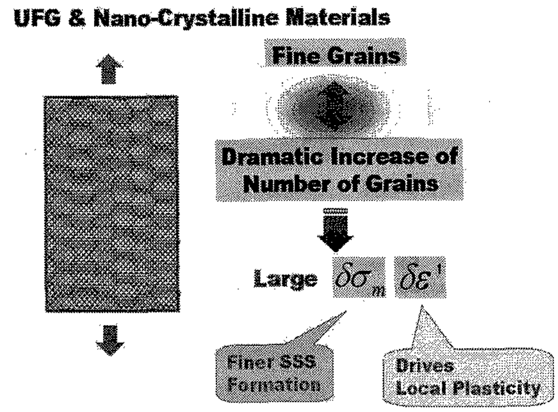


Fig. 14 Example of ultra-fine grained (UFG) or non-crystalline material yielding pronounced grain number effect.

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