Interaction and Multiscale Mechanics, Vol. 4, No. 2 (2011) 155-164
DOI: http://dx.doi.org/10.12989/imm.2011.4.2.155

Influence of grain interaction on lattice strain evolution in two-phase polycrystals

Tong-Seok Han*

School of Civil and Environmental Engineering, Yonsei University, Seoul 120-749, Korea

(Received November 11, 2010, Accepted February 26, 2011)

Abstract. The lattice strain evolution within polycrystalline solids is influenced by the crystal orientation and grain interaction. For multi-phase polycrystals, due to potential large differences in properties of each phase, lattice strains are even more strongly influenced by grain interaction compared with single phase polycrystals. In this research, the effects of the grain interaction and crystal orientation on the lattice strain evolution in a two-phase polycrystals are investigated. Duplex steel of austenite and ferrite phases with equal volume fraction is selected for the analysis, of which grain arrangement sensitivity is confirmed in the literature through both experiment and simulation (Hedström *et al.* 2010). Analysis on the grain interaction is performed using the results obtained from the finite element calculation based on the model of restricted slip within crystallographic planes. The dependence of lattice strain on grain interactions as well as crystal orientation is confirmed and motivated the need for more in-depth analysis.

Keywords: polycrystals; grain interaction; elasticity; plasticity; finite element method.

1. Introduction

Polycrystalline materials are used in wide range of engineering applications, but the detailed behavior at the micro-structural level has not been fully understood. To better understand the material behavior, further development of both experiment and modeling tools is required. Recent development of the high energy X-ray diffraction experiment techniques using synchrotron (e.g. Hedström *et al.* 2008) enabled further investigation of the material behavior in detail, but there are still increasing need for better modeling tool for validating the experiment and further analysis of the experimental data. In this research, findings from the experimental measurements of the lattice strains of a duplex (austenite - ferrite) steel are further investigated using the state-of-the-art modeling approach to provide more insights on the interpretation of the experimental data. Advanced models cannot be developed without experimental investigations, and experimental evidence can be further explained through modeling. This work is in line with pursuing the synergies of combining experiment and simulation to better understand the behavior of polycrystalline materials.

To improve mechanical properties multi-phase microstructures are often used. Multi-phase microstructures exhibit more complex and interesting behavior compared with single phase

* Assistant Professor, E-mail: tshan@yonsei.ac.kr

counterparts due to load/deformation partitioning between phases. One of the findings from the x-ray synchrotron experiment presented in Hedström *et al.* (2010) is the grain interactions on the lattice strain evolution. The experimental evidence showed that lattice strains evolved differently even for the grains with similar orientations. This work is motivated by the finding, and is intended to provide systematic approach for further analysis through modeling.

2. Experiment

The purpose of this work is to provide a simulation framework for the type of diffraction experiments as shown in Hedström *et al.* (2010), where the lattice strain evolution of a handful of two-phase crystals are measured. Detailed work on the experiment can be found in Hedström *et al.* (2010) and only a brief description is presented here. In situ three dimensional *x*-ray diffraction measurements rendered in-depth analysis of crystal behavior possible (Chung and Ice 1999, Margulies *et al.* 2002, Miller *et al.* 2008, Poulsen *et al.* 2001). Especially, lattice strain measurements of handful of crystals (Lienert *et al.* 2004, Hedström *et al.* 2010) accelerated the development and design of new materials and the identification of integrity of existing materials.

The single crystal level x-ray diffraction experiment was conducted on the duplex stainless steel SAF 2304 specimen from Outokumpu (Avesta, Sweden). The diffraction experiment was performed at the Advanced Photon Source (APS), Argonne, IL, USA. The length of the specimen was 22 mm, the width was 8 mm, and the thickness was 1.5 mm. From the Graindex analysis (Lauridsen *et al.* 2001) along with data reduction procedures, diffraction data for 15 single grains (8 austenite and 7 ferrite) were obtained. From the experiment, it was observed that grains with the similar orientations evolve to different loading states. This is a strong indication of the interaction among neighboring grains, and the response could be amplified due to large differences in material properties between phases. The source of the difference in lattice strain magnitude and spread is investigated using the state-of-the-art finite element simulation.

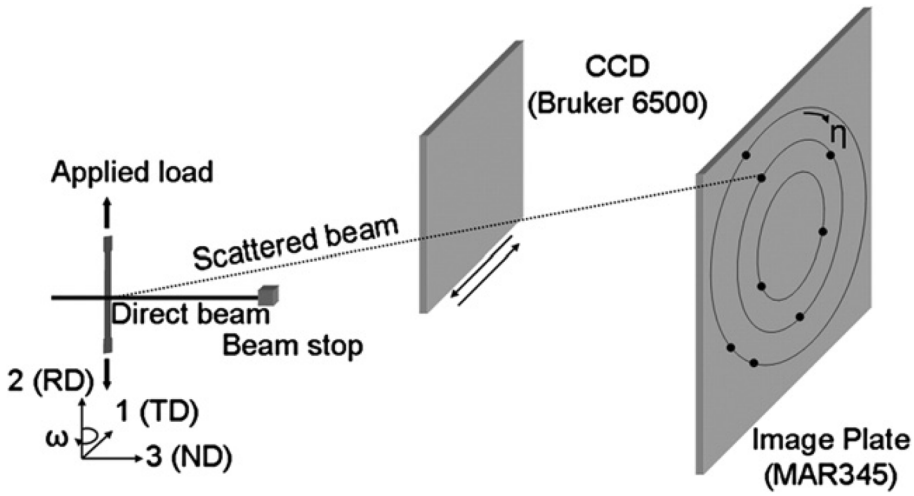

Fig. 1 High-energy x-ray diffraction setup (Reproduced from Hedström *et al.* (2010))

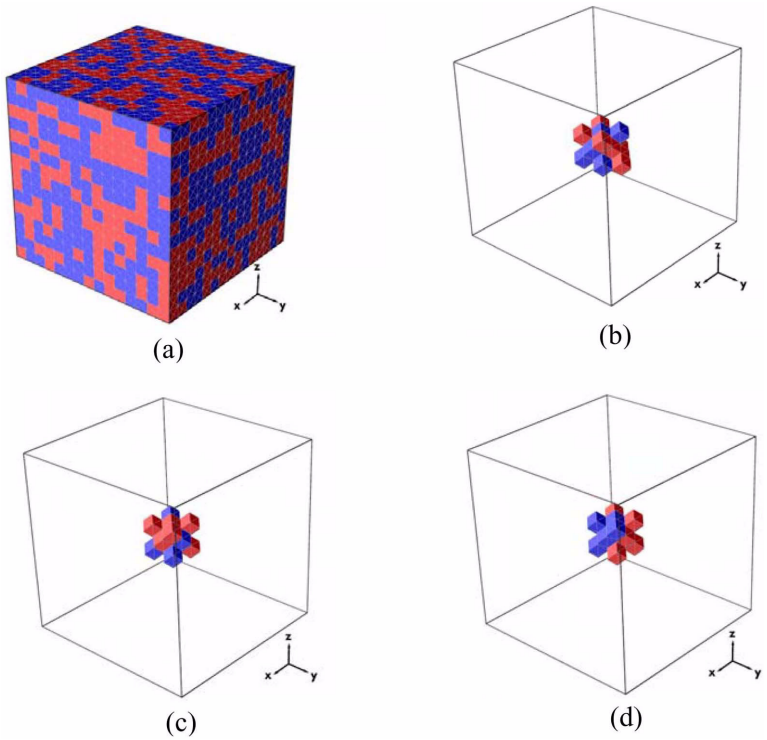

Fig. 2 Equal volume fraction two-phase finite element mesh and 15 grains embedded in the full mesh: (a) RVE, (b) Case 1, (c) Case 2, (d) Case 3

3. Modeling

The purpose of the simulation conducted in this research is to help identifying the influence of grain orientation and local environment on the lattice strain evolution within polycrystal aggregate. The single phase polycrystalline material is expected to produce less difference in the lattice strain evolution in the embedded grains than the two-phase material since the single phase material possesses less heterogeneous environment than the two-phase material does. The large difference in material properties of phases in the duplex steel should amplify the effect of the grain interaction, and it is adopted in this research.

To accomplish this task, a virtual specimen of representative volume element was generated (Fig. 2). In the middle of the representative volume (or virtual sample), 15 grains are embedded, where lattice strains are measured during the experiment. Since the information of grain arrangement of 15 grains is not available, the grains are assumed to be adjacent to one another. The effect of grain interaction from the neighboring grains is investigated by generating three different spatial arrangements of the 15 grains for the virtual specimen. The crystallographic orientations of the 15 grains are obtained from the experiment and are assigned to each grain. Random orientations are assigned to the rest of the grains within the virtual specimen as observed in the experiment. Unlike the experiment, initial strains are not applied to the virtual specimen. Since the main purpose of the simulation is to identify the differences that may arise from the grain interaction, the effect of the residual strains is removed.

In the finite element mesh presented in Fig. 2, each grain is represented by a dodecahedron with uniform surface shape and size. The dodecahedron is composed of 48 10-noded tetrahedral elements, where the same orientation and phase are assigned to represent a grain. In the mesh, there are a total of 2360 grains. The number of full grains, which are represented by a dodecahedron of 48 elements, is 1098, and the number of the partial grains is 1262. More natural grains shapes might be represented, for example, when the level set functions are used (Zhang *et al.* 2008), but it is out of the scope of the paper.

The finite element formulation adopted here (Marin and Dawson 1998a, 1998b) follows a standard procedure of minimizing the residual form of the equilibrium equation

$$R = \int_B \mathrm{tr}(\boldsymbol{\sigma}'^{T} \mathrm{grad}\,\Psi) dB + \int_B \pi \mathrm{div}\Psi dB + \int_{\partial B} \mathbf{t} \cdot \Psi \, d\Gamma + \int_B \mathbf{b} \cdot \Psi \, dB \tag{1}$$

where the Cauchy stress ($\boldsymbol{\sigma}$) is decomposed into deviatoric stress ($\boldsymbol{\sigma}'$) and pressure (π), $\mathbf{t}$ is the traction on the boundary of the body, $\mathbf{b}$ is the body force, and Ψ is the weight function. Adopting the Bubnov-Gelerkin method, the same interpolation function used for the displacement field is used for Ψ. By discretizing the domain and enforcing $R \cong 0$ of Eq. (1), the equation reduces to a matrix equation for nodal velocities. Extension of this formulation including the efficient solution algorithm can be found in Matou and Maniatty (2009).

An elasto-viscoplastic constitutive model (Marin and Dawson 1998a) is used. The elastic behavior is defined by Hooke's law relating Kirchhoff stress (τ) and elastic strain with elastic moduli, and small elastic strain is assumed for the formulation. For the plastic behavior, the shear strain rate ($\dot{\gamma}^{\alpha}$) on a crystallographic slip plane (α) is expressed as a function of the resolved shear stress (τ^{α}) using a power law (Hutchinson 1976)

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{|\tau^{\alpha}|}{g^{\alpha}} \right)^{\frac{1}{m}} \mathrm{sgn}(\tau^{\alpha}) \tag{2}$$

where $\dot{\gamma}_0$ is reference shear strain rate, m is a rate sensitivity parameter, and g^{α} is slip system strength. Hardening of the crystallographic slip system strength is evolved according to the modified Voce law (Voce 1948) as

$$\dot{g}^{\alpha} = h_0 \left(\frac{g_s - g^{\alpha}}{g_s - g_0} \right)^{n} \dot{\gamma} \tag{3}$$

where g_s is the saturated slip system strength, g_0 is the initial slip system strength, h_0 and n are modeling parameters. $\dot{\gamma}$ is the sum of absolute values of the shear strain rate ($\dot{\gamma}^{\alpha}$) for all crystallographic slip systems. Using the multiplicative decomposition, the elastic and plastic behaviors are combined.

Symmetric boundary conditions are assigned to the three hidden surfaces in the virtual specimen. Tension (in z direction) is applied at the top surface, and two other surfaces were remained free. The lattice strains are calculated up to 0.02 applied strain with the loading rate of $10^{-4} s^{-1}$. The modeling parameters are determined by fitting the macroscopic stress-strain curve with further adjustment to match the lattice strain levels. The parameter calibration procedure is presented in Hedström *et al.* (2010), and the same parameters are used for the analysis presented here. The elastic moduli obtained from Kelly *et al.* (2000) as well as the viscoplastic parameters are presented

Table 1 Modeling parameters and elastic moduli

Phase	Slip system parameters						Elastic moduli (GPa)		
	h_0 (MPa)	g_0 (MPa)	g_s (MPa)	$\dot{\gamma}_0$ (s^{-1})	m	n	c_{11}	c_{12}	c_{44}
Austenite	600.0	136.5	476.0	1.0	0.02	1.0	197.5	124.5	122.0
Ferrite	400.0	111.3	210.0	1.0	0.02	1.0	237.4	134.7	116.4

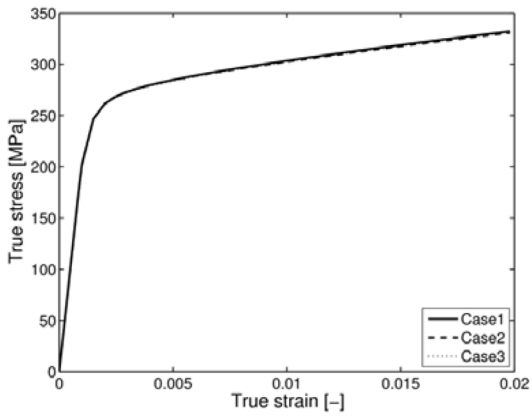

Fig. 3 Macro-scale stress-strain curves of microstructual mesh of the three grain arrangements shown in Fig. 2

in Table 1. The simulations are conducted on 30 CPU cores on a cluster computer at the Korean Institute of Science and Technology information (KISTI).

4. Analysis

The macro-scale response of the three cases of grain rearrangements are presented in Fig. 3. The stress-strain curves are almost lying on top of each other. The macro-scale level perturbation induced by the rearrangement of 15 grains embedded in more than 1000 grains should not be significant, which is confirmed from the macro-scale response shown in the figure. However, the local perturbation should exist through different grain interactions from different grain topology, and is described next by investigating lattice strain evolution at the micro-scale single crystal level.

Through the simulation, lattice strains from the specified 15 grains are monitored. Among the grains, plots of the lattice strain evolution of one austenite and one ferrite grains are presented in Figs. 4 and 5. Other grains also show similar results although there are some variations in responses. The orientation of the austenite and ferrite grains presented in the figures are (0.505, -0.227, 0.414) and (0.494, 0.092, -0.206) in Rodrigues vector from (Kocks *et al.* 1998), respectively. In the experiment, lattice strain evolutions of grains with a similar orientation are monitored for a given loading history, while, in simulation, lattice strain evolution of the same grain from three arrangements are obtained. To clearly identify the source of differences in the lattice strain level from the simulation, three independent simulations with different grain arrangements of the same crystal orientation set are performed.

In Fig. 4, lattice strain evolutions of the austenite grain from three grain arrangement (Fig. 2) are presented. Although the grain with the same orientation from the three arrangements is monitored,

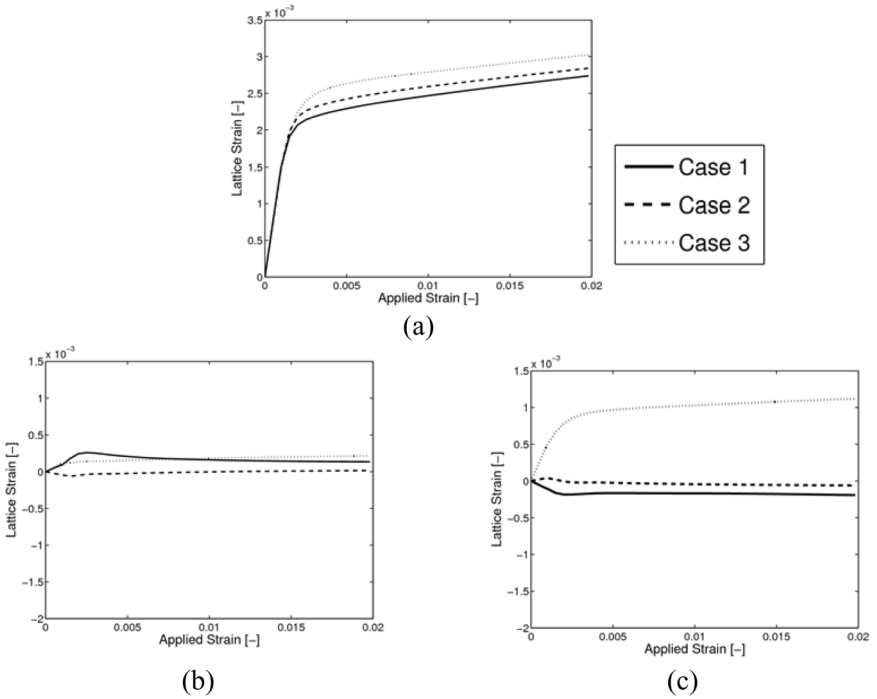

Fig 4. Lattice strain of an austenite grain: (a) ε_{zz}, (b) ε_{xx}, (c) ε_{xy}

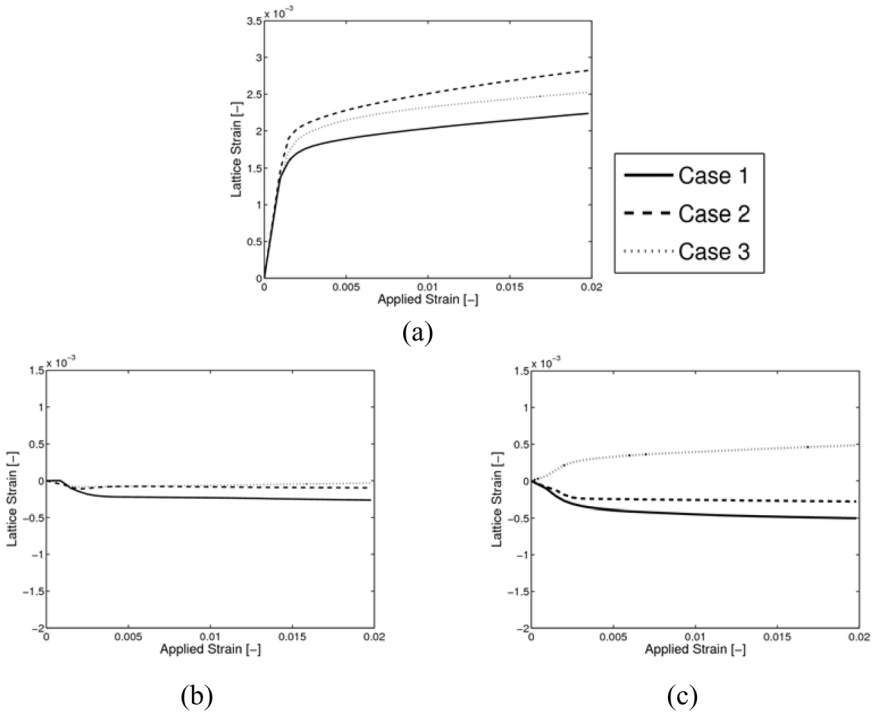

Fig. 5 Lattice strain of a ferrite grain: (a) ε_{zz}, (b) ε_{xx}, (c) ε_{xy}

the lattice strain levels are different among the three cases. The same trend is obtained for ferrite grains, and an example is presented in Fig. 5. For both cases, the difference of the lattice strains can be clearly identified. The yielding occurs around 0.002 of applied strain for the austenite grain, where the slope of the lattice (elastic) strain relationship of ε_{zz} changes. The slope change of lattice strain ε_{zz} of ferrite grains occurs around 0.001, which can be also identified by a slight slope change in the elastic regime of the lattice strain behavior for the austenite grain.

Transverse lattice strains (ε_{xx}) in the austenite grain (Fig. 4) are mainly positive although longitudinal lattice strains (ε_{zz}) are positive, which should be attributed to the grain interaction from the neighboring grains. Transverse lattice strains in ferrite grain (Fig. 5) are all negative. For both grains, the lattice strains in some cases are reversed as yielding occurs. This is an indication of the grain interaction and the sudden stress direction change upon yielding.

The lattice strains (ε_{xy}) show similar trend as the longitudinal lattice strains do. The rate of lattice strain change substantially deceases as grains yield. In the results presented here, the signs of the lattice strains are different among three arrangements. This is another indication that the grain interaction can change the stress direction.

In this research, a grain represented by a dodecahedron is composed of 48 elements, and each element can develop its strain through interactions with neighboring elements. This mimics the actual physical behavior in a real material. Hence, although not significant, the lattice strains within a grain vary and the standard deviations of the lattice strains can provide information on the grain interactions. Figs. 6 and 7 showed that the standard deviations of lattice strains are about one order of magnitude lower than the lattice strain values. It is interesting to note that the magnitudes of standard deviations for three strain components are similar except for the standard deviation of ε_{xy} for the ferrite grain. As in the case for the lattice strains, there are differences in the standard deviations of lattice strains for each grain of three arrangements. Depending on the component, the standard deviation increases or decreases as the applied loading increases. It can be also noted that the local maximum of standard deviation occurs in many cases around the yielding point. This is an indication of progressive yielding of elements that constitute a dodecahedral grain in the modeling.

The evolution of the lattice strain tensor is illustrated in Fig. 8, where the strain tensor is visualized using a strain "jack" (Han and Dawson 2005) with the principal strains and their directions. The principal strain directions are represented by the three orthogonal cylinders from the eigenvectors of the strain tensor. The principal strains, eigenvalues of the strain tensor are mapped on to the corresponding cylinders of principal directions. In Fig. 8, strain tensors of an ferrite crystal at the applied strains of 0.08, 0.6, and 1.7% are illustrated for three cases of grain arrangement. The strain levels are selected for monitoring strain evolution before and after yielding and when full plasticity is developed. The strains directions among three cases are clearly different for both elastic (0.08% strain) and plastic (0.6% and 1.7% strains) cases. The strain states are not identical even for the elastic range due to interactions between crystals with anisotropic elastic constants and different crystal orientations. Once the plasticity develops, the compatibility requirement among grains determines the favorable slip systems, and this may results in different polyslip modes (Barton *et al.* 1999, Kocks 1960, Ritz *et al.* 2010). It can be also noticed that the strain direction is changed as the plasticity develops for each case. During plastic flow, the lattice strain direction is changed as the stress direction is moving toward the single crystal yield stress vertex to accommodate the compatible deformation mode between anisotropic crystals through polyslip (Kocks 1960). The direction change of the strain tensor is due to the fact that the stress direction is moving toward the vertex of the single crystal yield surface and this is confirmed for the two-phase materials.

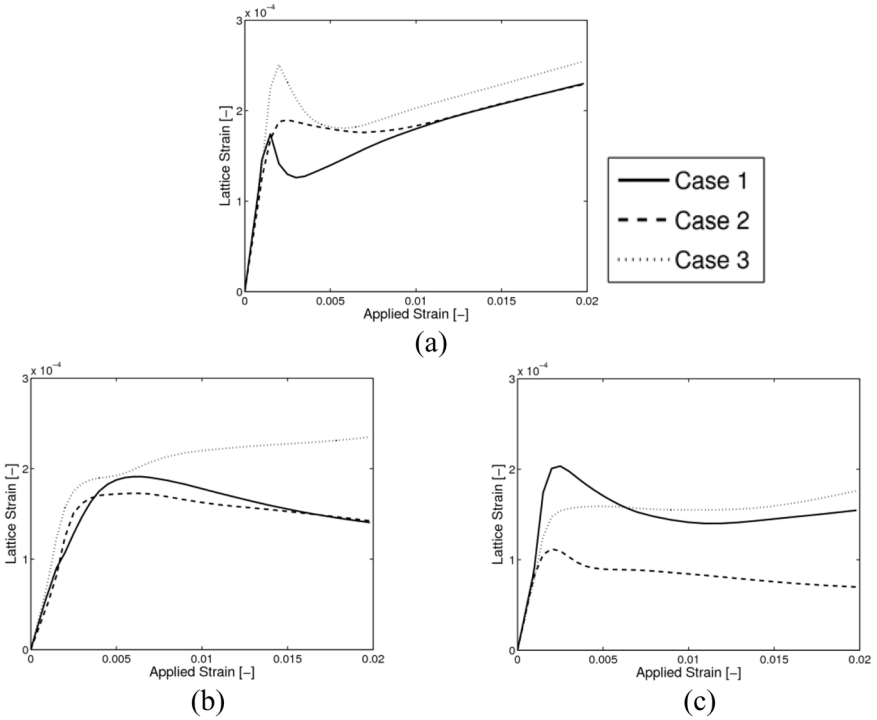

Fig. 6 Standard deviation of lattice strains of an austenite grain: (a) ε_{zz}, (b) ε_{xx}, (c) ε_{xy}

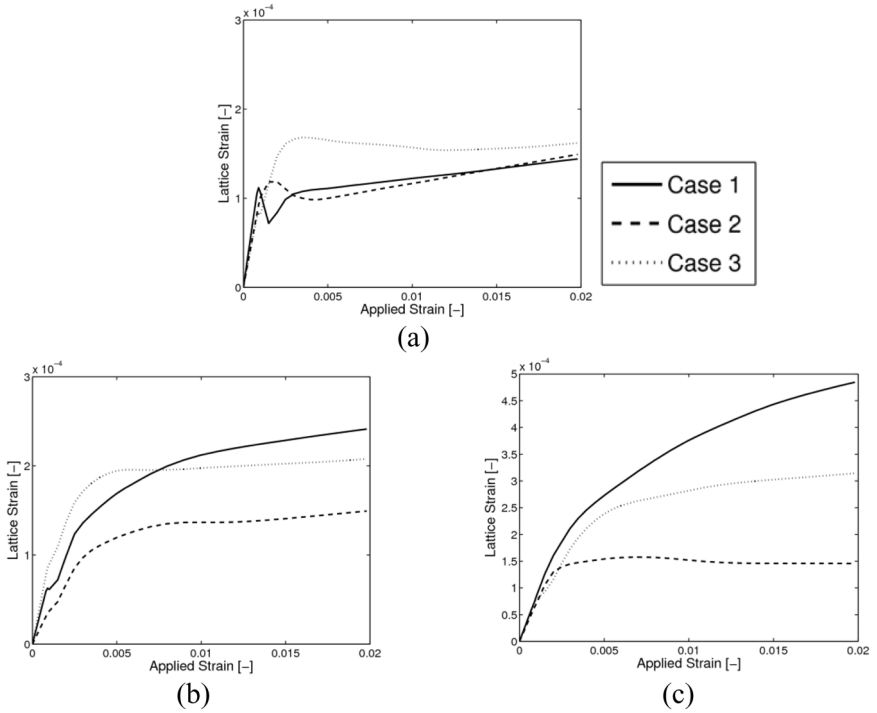

Fig. 7 Standard deviation of lattice strains of a ferrite grain: (a) ε_{zz}, (b) ε_{xx}, (c) ε_{xy}

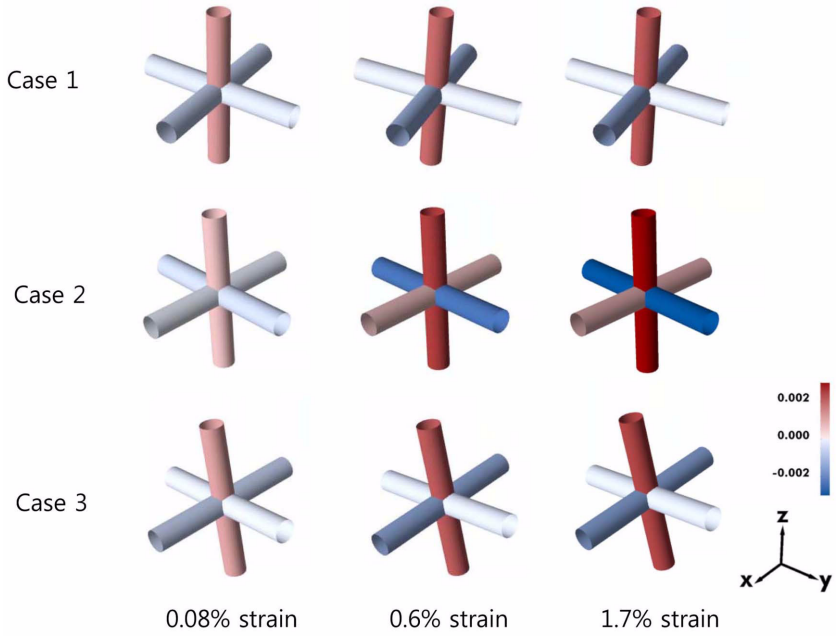

Fig. 8 Lattice strain evolution of a ferrite grain as a function of the applied macro-scale strain (Note: The numbers on the colorbar stands for strains of no unit.)

5. Conclusions

The effect of neighboring grains on the lattice strain evolution in a two-phase polycrystalline solid was investigated using the finite element analysis. From the simulation of the three grain arrangements of the same set of crystal orientations, it was evident that the lattice strains evolve differently due to the grain interactions. The standard deviations of the lattice strains also showed that the existence of grain interactions. The standard deviations are amplified upon yielding of each grain, and the standard deviations decrease as plasticity develops. These evolution patterns of the lattice strains and their standard deviations strongly suggest the dependence on grain interactions as well as crystal orientations. The effect of the grain interactions on the lattice strain evolution of a single crystal was also confirmed by the visualization of the lattice strain tensors for three cases. The lattice strain tensor directions are changed upon yielding and stabilized as the full plasticity develops. This indicates the progressive yielding of a crystal, which contributes to the complex grain interactions.

These results motivate a systematic analysis on the lattice strain/stress direction evolution compared with the single crystal yield vertex combined with the grain misorientation relative to the surrounding grains and phase interactions of strongly dissimilar properties.

Acknowledgments

This work was supported by the Korea Research Foundation Grant funded by the Korean

Government (MOEHRD) KRF-2008-331-D00006, in which parallel finite element calculations were performed by using the supercomputing resource of the Korean Institute of Science and Technology information (KISTI).

References

Barton, N., Dawson, P. and Miller, M. (1999), "Plastic stress-strain relations of fcc polycrystalline metals hardening according to the Taylor rule", *J. Eng. Mater. Technol.*, **12**, 230-239.

Chung, J.S. and Ice, G. (1999), "Automated indexing for texture and strain measurement with broadband pass *x*-ray microbeams", *J. Appl. Phys.*, **86**(9), 5249-5255.

Han, T.S. and Dawson, P.R. (2005), "Lattice strain partitioning in a two-phase alloy and its redistribution upon yielding", *Mater. Sci. Eng. A*, **405**, 18-33.

Hedström, P., Lienert, U.L., Almer, J. and Odén, M. (2008), "Elastic strain evolution and ε-martensite formation in individual austenite grains during in situ loading of a metastable stainless steel", *Mater. Lett.*, **62**, 338-340.

Hedström, P., Han, T.S., Lienert, U.L., Almer, J. and Odén, M. (2010), "Load partitioning between single bulk grains in a two-phase duplex stainless steel during tensile loading", *Acta Mater.*, **58**, 734-744.

Hutchinson, J.W. (1976), "Bounds and self-consistent estimates for creep of polycrystalline materials", *Proceedings of Royal Society of London, Series A*, **348**(1652), 101-127.

Kelly, A., Groves, W. and Kidd, P. (2000), *Crystallography and crystal defects*, John Wiley & Sons Ltd., Revised edition.

Kocks, U.F. (1960), "Polyslip in single crystals", *Acta Metal.*, **8**(6), 345-352.

Kocks, U.F., Tomé, C.N. and Wenk, H.R. (1998), *Texture and anisotropy*, Cambridge Press, Cambridge.

Lauridsen, E.M., Schmidt, S., Suter, R.M. and Poulsen, H.F. (2001), "Tracking: a method for structural characterization of grains in powders or polycrystals", *J. Appl. Crystallogr.*, **34**, 744-750.

Lienert, U., Han, T.S., Almer, J., Dawson, P.R., Leffers, T., Margulies, L., Nielsen, S.F., Poulsen, H.F. and Schmidt, S. (2004), "Investigating the effect of grain interaction during plastic deformation of copper", *Acta Mater.*, **52**, 4461-4467.

Margulies, L., Lorentzen, T., Poulsen, H.F. and Leffers, T. (2002), "Strain tensor development in a single grain in the bulk of a polycrystal under loading", *Acta Mater.*, **50**(7), 1771-1779.

Marin, E.B. and Dawson, P.R. (1998a), "On modelling the elasto-viscoplastic response of metals using polycrystal plasticity", *Comput. Method. Appl. M.*, **165**, 1-21.

Marin, E.B. and Dawson, P.R. (1998b), "Elastoplastic finite element analyses of metal deformations using polycrystal constitutive models", *Comput. Method. Appl. M.*, **165**, 23-41.

Matous, K. and Maniatty, A.M. (2009), "Multiscale modeling of elasto-viscoplastic polycrystals subject to finite deformation", *Interact. Multiscale Mech.*, **2**(4), 375-396.

Miller, M.P., Park, J.S., Dawson, P.R. and Han, T.S. (2008), "Measuring and modeling distributions of stress state in deforming polycrystals", *Acta Mater.*, **56**, 3927-3939.

Poulsen, H.F., Nielsen, S.F., Schmidt, S., Lauridsen, E.M., Suter, R.M., Lienert, U., Margulies, L., Lorentzen, T. and Jensen, D.J. (2001), "Three-dimensional maps of grain boundaries and the stress state of individual grains inpolycrystals and powders", *J. Appl. Crystallogr.*, **34**, 751-756.

Ritz, H., Dawson, P.R. and Marin, T. (2010), "Analyzing the orientation dependence of stresses in polycrytals using vertices of the single crystal yield surface and crystallographic fibers of orientation space", *J. Mech. Phys. Solids*, **58**, 54-72.

Voce, E. (1948), "The relationship between stress and strain for homogeneous deformation", *J. Institute Metal.*, **74**, 537-562.

Zhang, X., Chen, J.S. and Osher, S. (2008), "A multiple level set method for modeling grain boundary evolution of polycrystalline materials", *Interact. Multiscale Mech.*, **1**(2), 191-209.