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Phase-field Modeling of Microstructures and Rapid Image-Based Calculation of Stress-Strain Curve

Toshiyuki Koyama

Department of Materials Science and Engineering
Nagoya Institute of Technology

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Material properties ⇔ Microstructures

Phase-field method (Direct calculation of microstructure morphologies)

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Image-based calculation of material properties

(Direct calculation of material properties using the microstructure morphologies)

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Effective strategy for materials design

(Images obtained from PF method are utilized as input data for image-based calculations)

Background:

High tensile strength steel such as a dual phase (DP) steel is one of the key materials on the development of electric vehicle for the body weight saving, where the second phase morphology crucially influences the mechanical properties.

Objective:

To propose the rapid Image-based calculation method of mechanical property (stress-strain curve) by using the microstructure data obtained from the phase-field simulations. (This study is a practical industrial application of PF method.)

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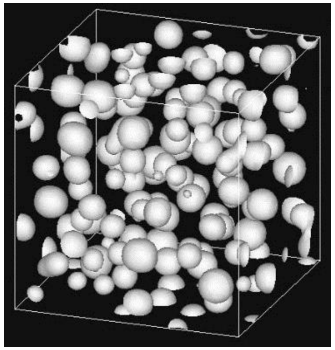
Several types of two-phase microstructures

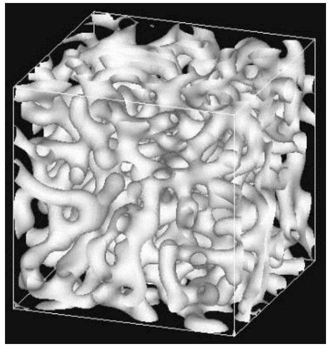
(Qualitative PF calculation: we don't consider the specific material.)

Two-phase Microstructures:

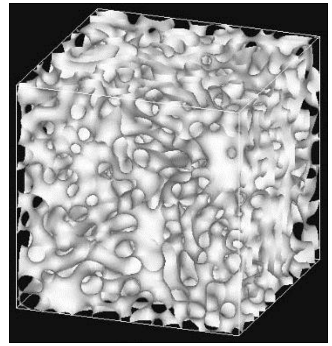
$f_1 = 0.1$



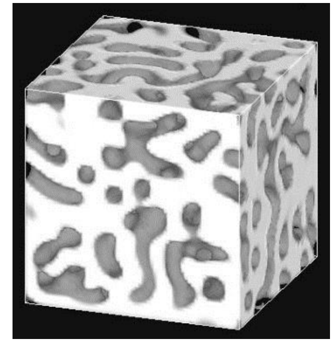
$f_1 = 0.3$



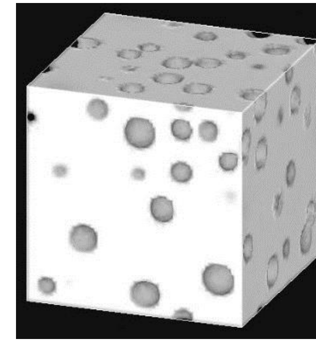
$f_1 = 0.5$



$f_1 = 0.7$

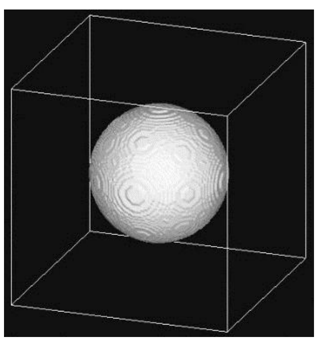


$f_1 = 0.9$



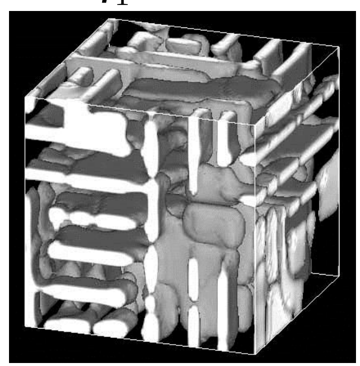
Mottled structure (Isotropic morphology)

$f_1 = 0.3$



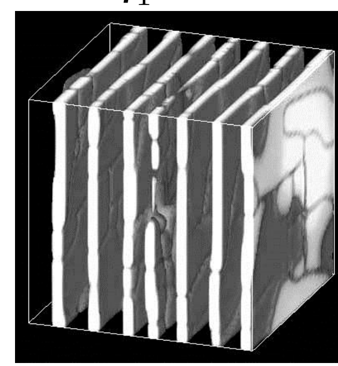
Sphere
(Single inclusion)

$f_1 = 0.3$



Modulated structure

$f_1 = 0.3$



Layered structure

(Anisotropic morphology)

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Secant method [G.J.Weng: J. Mech. Phys. Solid, 38(1990), 419.]

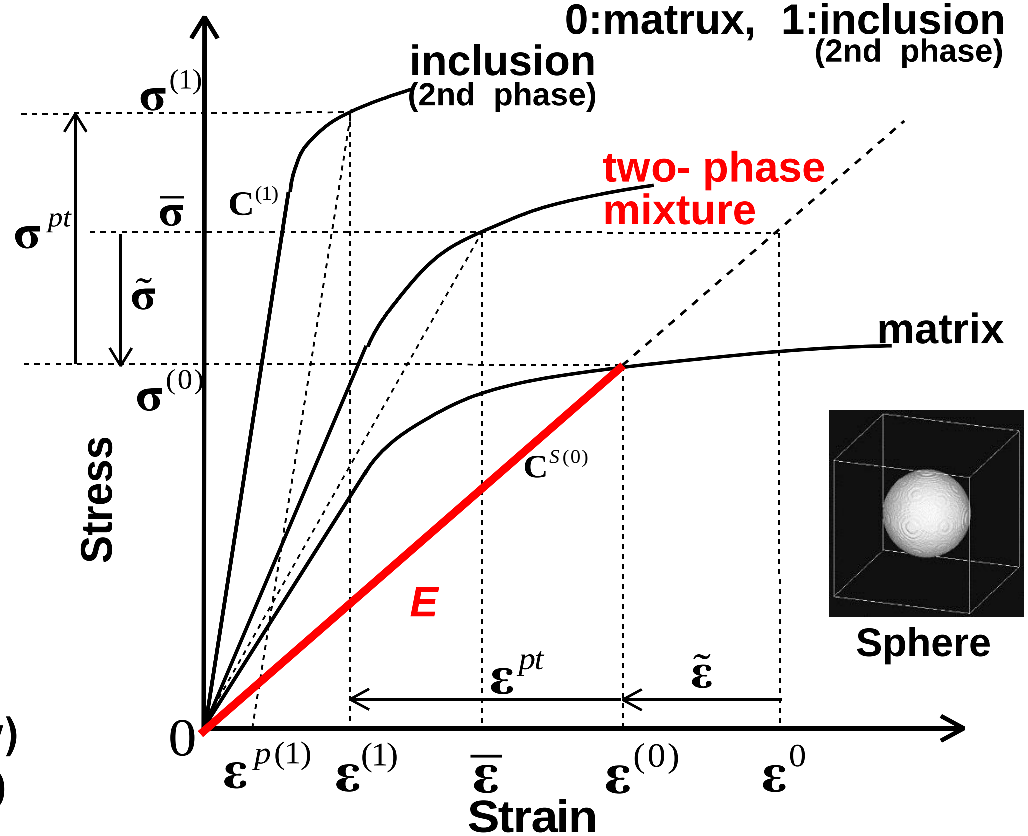
Phenomenological method to calculate the S-S curve of two-phase composite

Assumptions:

(1) Both two S-S curves of matrix phase and 2nd phase are given in advance.

(2) Mean field theory by Mori and Tanaka (Micromechanics).

(3) Secant elastic moduli
Plastically deformed matrix
→ Elastic medium having secant moduli



Sphere

(Hooke's law)

$$\boldsymbol{\varepsilon}^0 = (\mathbf{C}^{S(0)})^{-1}\bar{\boldsymbol{\sigma}}, \quad \boldsymbol{\sigma}^{(0)} = \mathbf{C}^{S(0)}(\boldsymbol{\varepsilon}^0 + \tilde{\boldsymbol{\varepsilon}})$$

$$\boldsymbol{\sigma}^{(1)} = \mathbf{C}^{(1)}(\boldsymbol{\varepsilon}^0 + \tilde{\boldsymbol{\varepsilon}} + \boldsymbol{\varepsilon}^{pt} - \boldsymbol{\varepsilon}^{p(1)}) = \mathbf{C}^{S(0)}[\boldsymbol{\varepsilon}^0 + \tilde{\boldsymbol{\varepsilon}} + \boldsymbol{\varepsilon}^{pt} - (\boldsymbol{\varepsilon}^{p(1)} + \boldsymbol{\varepsilon}^*)]$$ (equivalent inclusion)

$$\boldsymbol{\varepsilon}^{pt} = \underline{\mathbf{S}^{S(0)}}(\boldsymbol{\varepsilon}^{p(1)} + \boldsymbol{\varepsilon}^*)$$ (Eshelby tensor ← mechanical equilibrium equation)

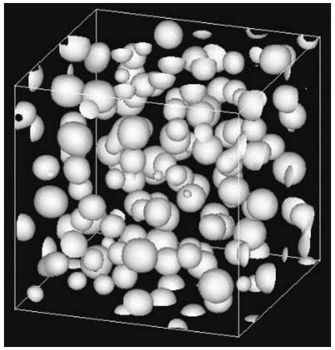
$$\bar{\boldsymbol{\sigma}} = f_0\boldsymbol{\sigma}^{(0)} + f_1\boldsymbol{\sigma}^{(1)}, \rightarrow \tilde{\boldsymbol{\varepsilon}} = -f_1(\mathbf{S}^{S(0)} - \mathbf{I})(\boldsymbol{\varepsilon}^{p(1)} + \boldsymbol{\varepsilon}^*)$$

$$\bar{\boldsymbol{\varepsilon}} = f_0\boldsymbol{\varepsilon}^{(0)} + f_1\boldsymbol{\varepsilon}^{(1)} = \boldsymbol{\varepsilon}^0 + f_1(\boldsymbol{\varepsilon}^{p(1)} + \boldsymbol{\varepsilon}^*)$$

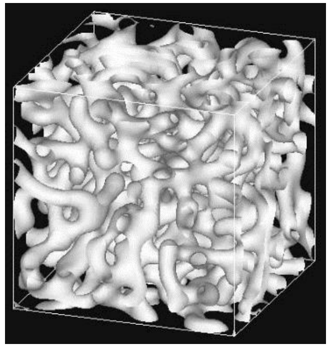
(mean field theory)

Modified secant method which can be applied to arbitrary morphology of microstructure [T.Koyama, ISIJ International, 52(2012),723.]

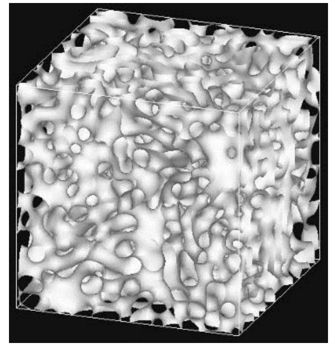
$f_1 = 0.1$



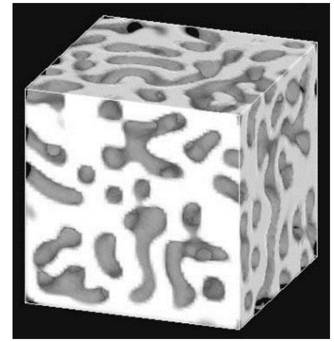
$f_1 = 0.3$



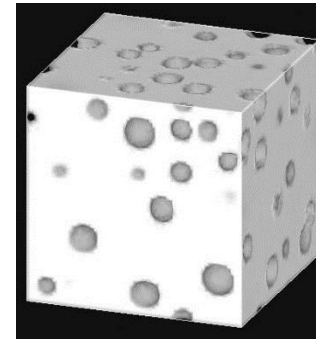
$f_1 = 0.5$



$f_1 = 0.7$

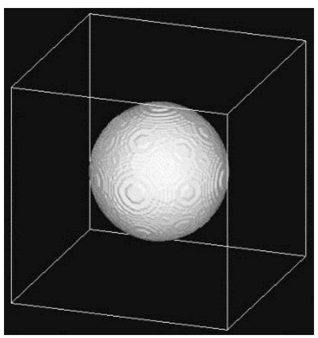


$f_1 = 0.9$



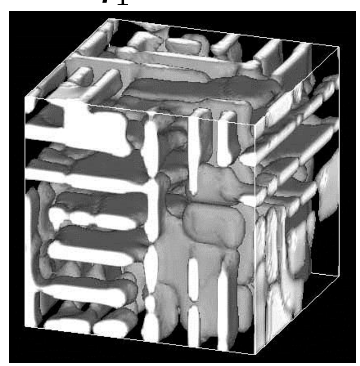
Mottled structure

$f_1 = 0.3$



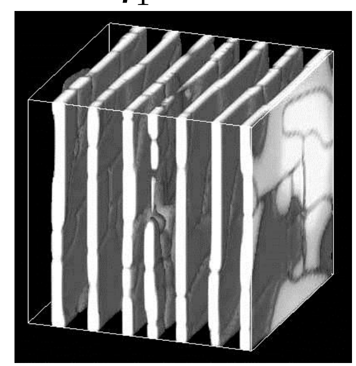
Sphere

$f_1 = 0.3$



Modulated structure

$f_1 = 0.3$



Layered structure

Calculation of S-S curves dependent on the microstructure

- **Case 1: Tensile strength of 2nd phase is low**
- **Case 2: Tensile strength of 2nd phase is high**

Case 1: Tensile strength of 2nd phase is low, i.e. plastic deformation is dominant in both phases.（matrix：ferrite, 2nd phase：pearlite）

Ferrite: $\sigma = 744(0.002 + \varepsilon^p)^{0.2345}$ [MPa]

Pearlite: $\sigma = 1160(0.001 + \varepsilon^p)^{0.1630}$ [MPa]

$E_0 = 200$[GPa], $\nu_0 = 0.3$

[Rudiono and Y.Tomota: Acta Mater., 45(1997), 1923]

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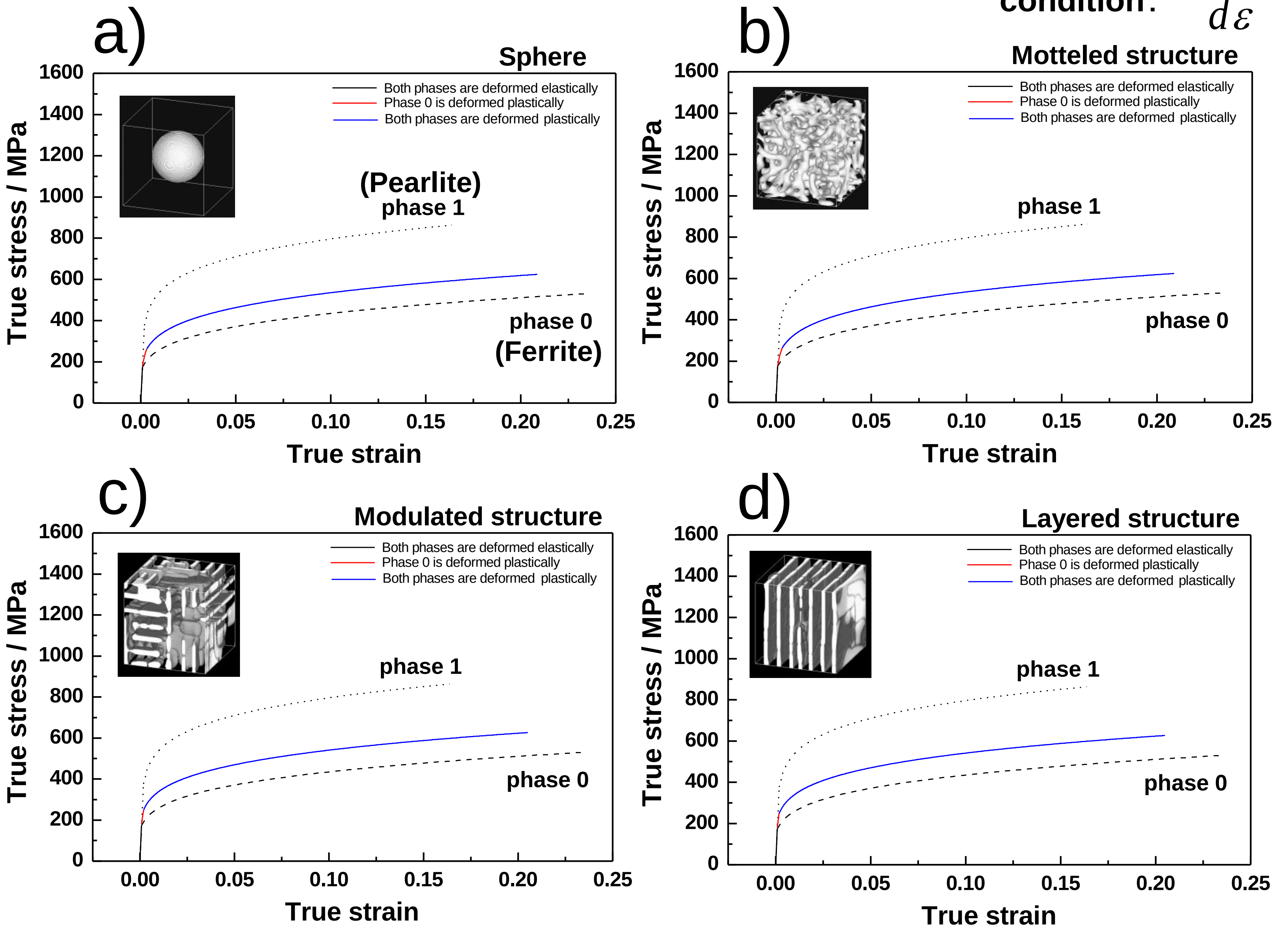
Constriction condition: $\dfrac{d\sigma}{d\varepsilon} = \sigma$



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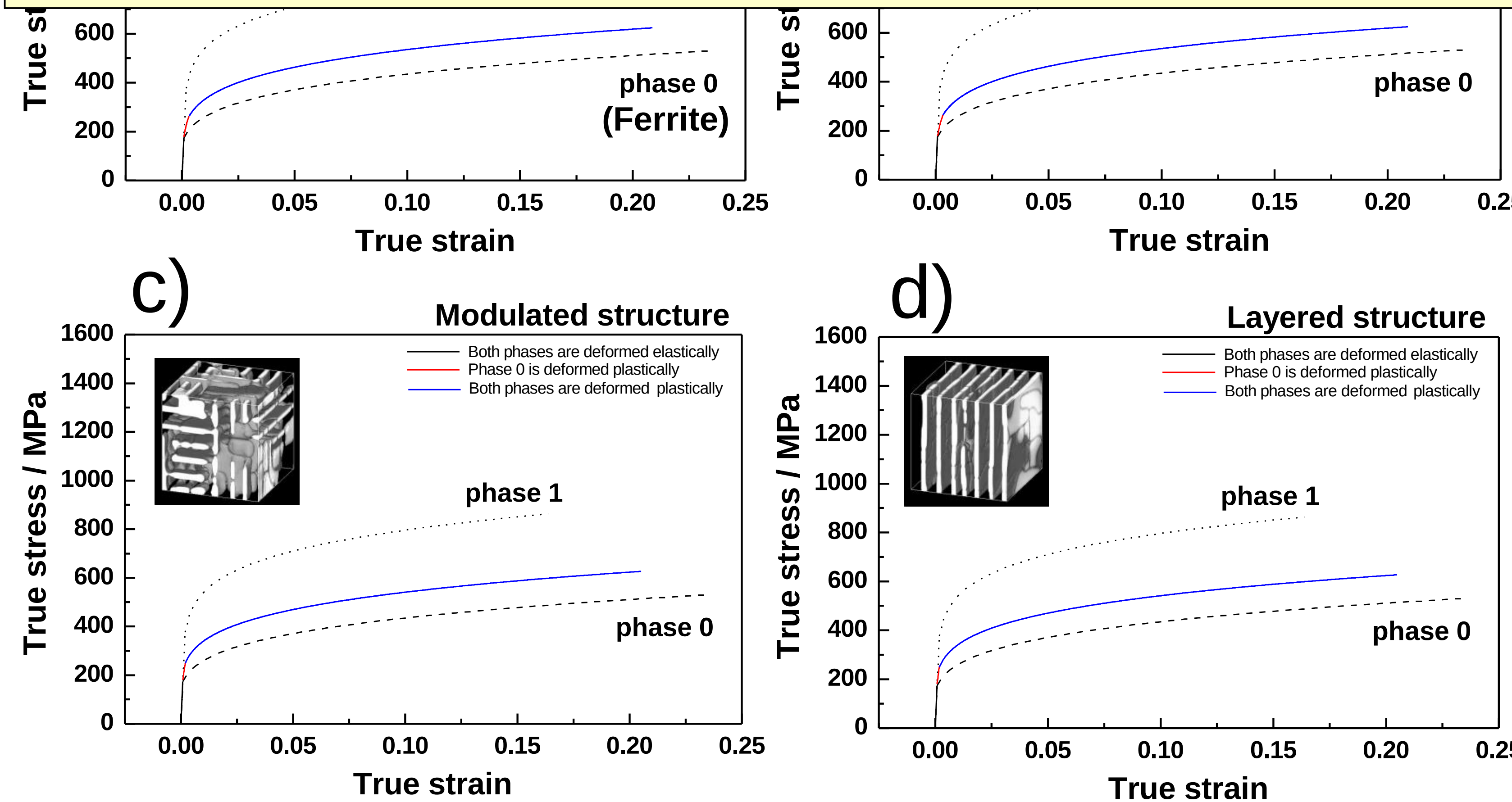
Constriction condition: $\frac{d\sigma}{d\varepsilon} = \sigma$

When the plastic deformation is dominant in both phases, the shape of S-S curve does not depend on the morphology of microstructure. It is determined by the volume fraction of 2nd phase.



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Case 2: Tensile strength of 2nd phase is high, i.e. 2nd phase is hard.（matrix：ferrite, 2nd phase：bainite）

Ferrite： $\sigma = 744(0.002 + \varepsilon^{p})^{0.2345}$ [MPa]

Bainite： $\sigma = 1643(0.0005 + \varepsilon^{p})^{0.0751}$ [MPa]

$E_1 = 200$[GPa], $\nu_1 = 0.3$

[Rudiono and Y.Tomota: Acta Mater., 45(1997), 1923]

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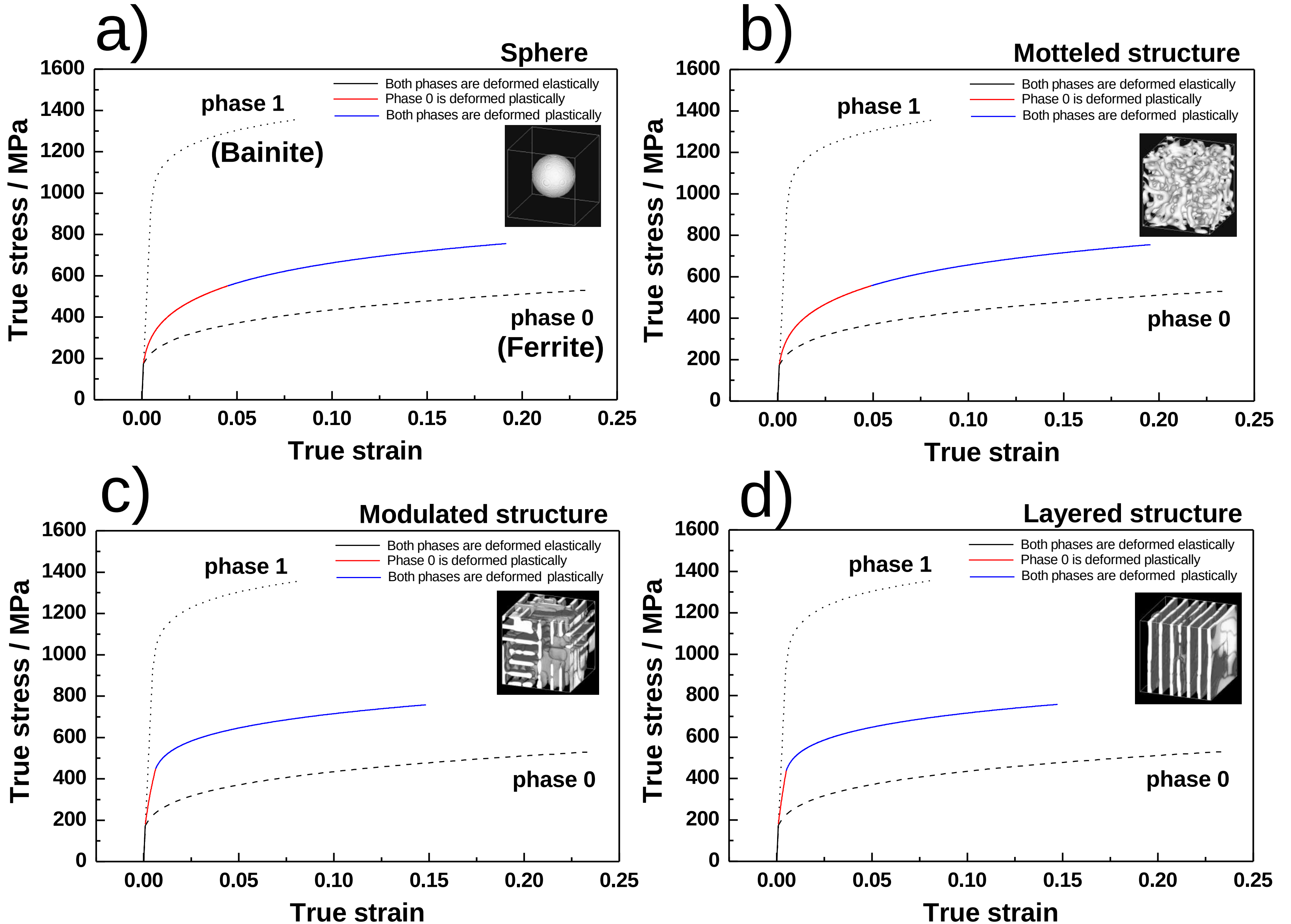

SS-curve depends on the morphology of microstructure, the work- hardening rate increases and the elongation decreases when the morphology of microstructure changes from isotropic to anisotropic.

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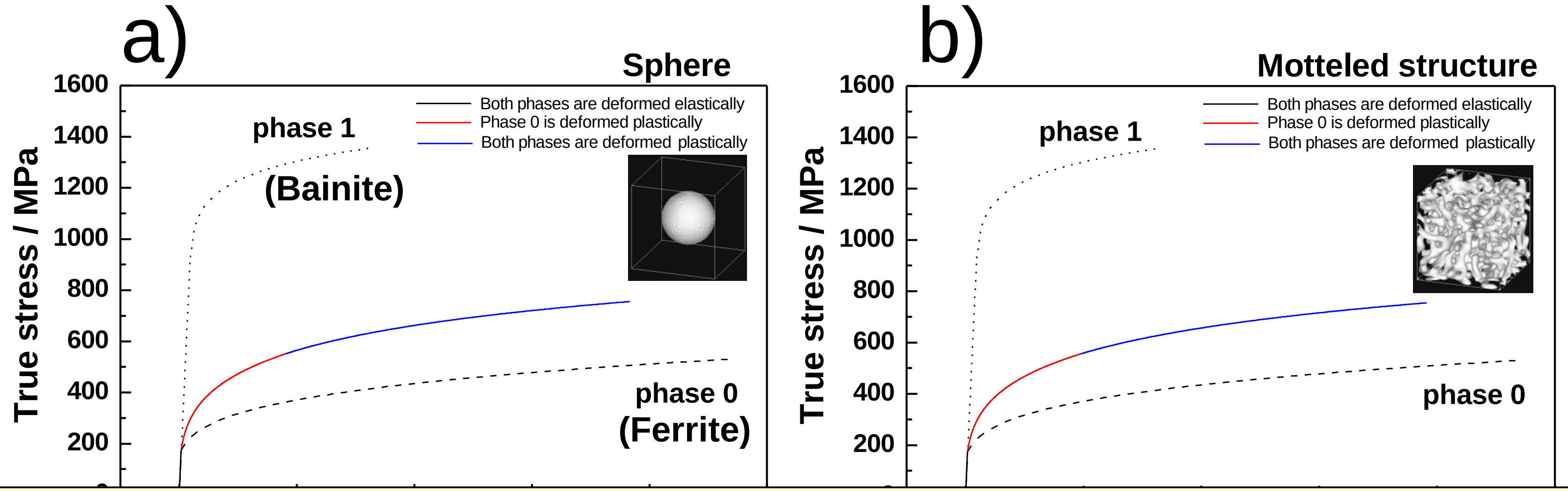
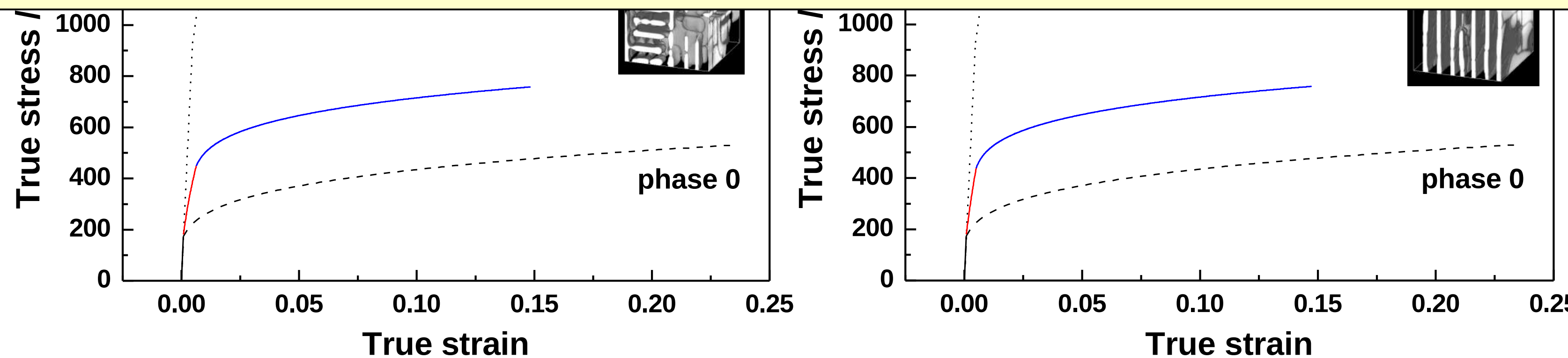


In the case that the contribution of the elastic deformation of the 2nd phase is large, the shape of S-S curve depends not only on the volume fraction of 2nd phase but also on the morphology of microstructure.



SS-curve depends on the morphology of microstructure, the work- hardening rate increases and the elongation decreases when the morphology of microstructure changes from isotropic to anisotropic.

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The change of stress-strain curve during spheroidization of lamella structure

－ Introduction of a topological parameter －

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Spheroidization of lamella structure

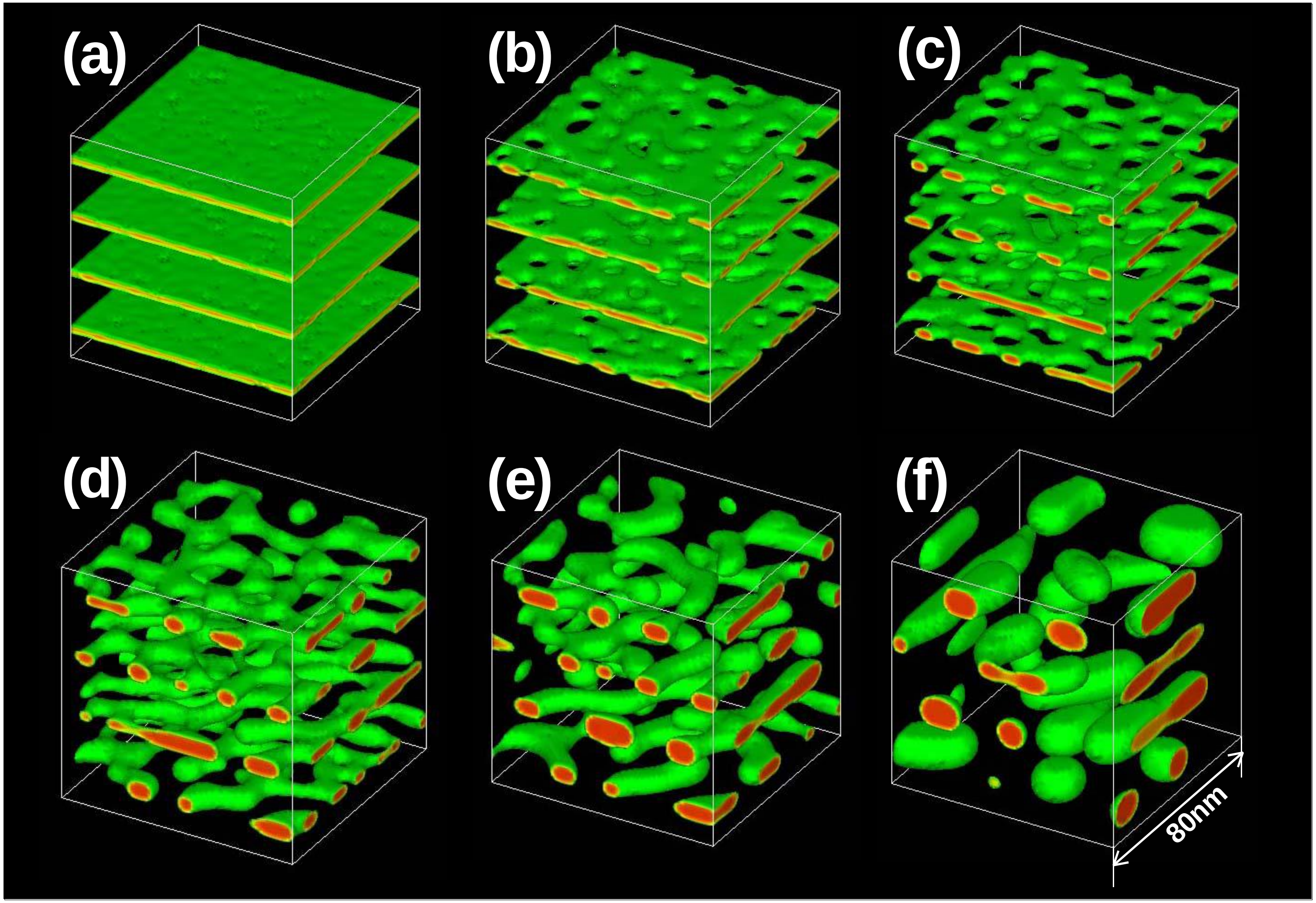

Fig.1 Three-dimensional phase-field simulation of the spheroidization of lamella structure, (a) *t*'=0, (b) *t*'=50, (c) *t*'=100, (d) *t*'=250, (e) *t*'=500 and (f) *t*'=2000.

Parameter values in Swift equation

$$\sigma = A(B + \varepsilon^{p})^{N} \quad [\mathrm{MPa}]$$

$$E_0 = 200[\mathrm{GPa}], \quad \nu_0 = 0.3$$

	A	*B*	*N*
Ferrite[1]	744	0.002	0.2345
Pearlite[1]	1160	0.001	0.163
Bainaite[1]	1643	0.0005	0.0751
Martensite	1550	10^{-7}	0.04

(1) Rudiono and Y.Tomota: Acta Mater., 45(1997), 1923

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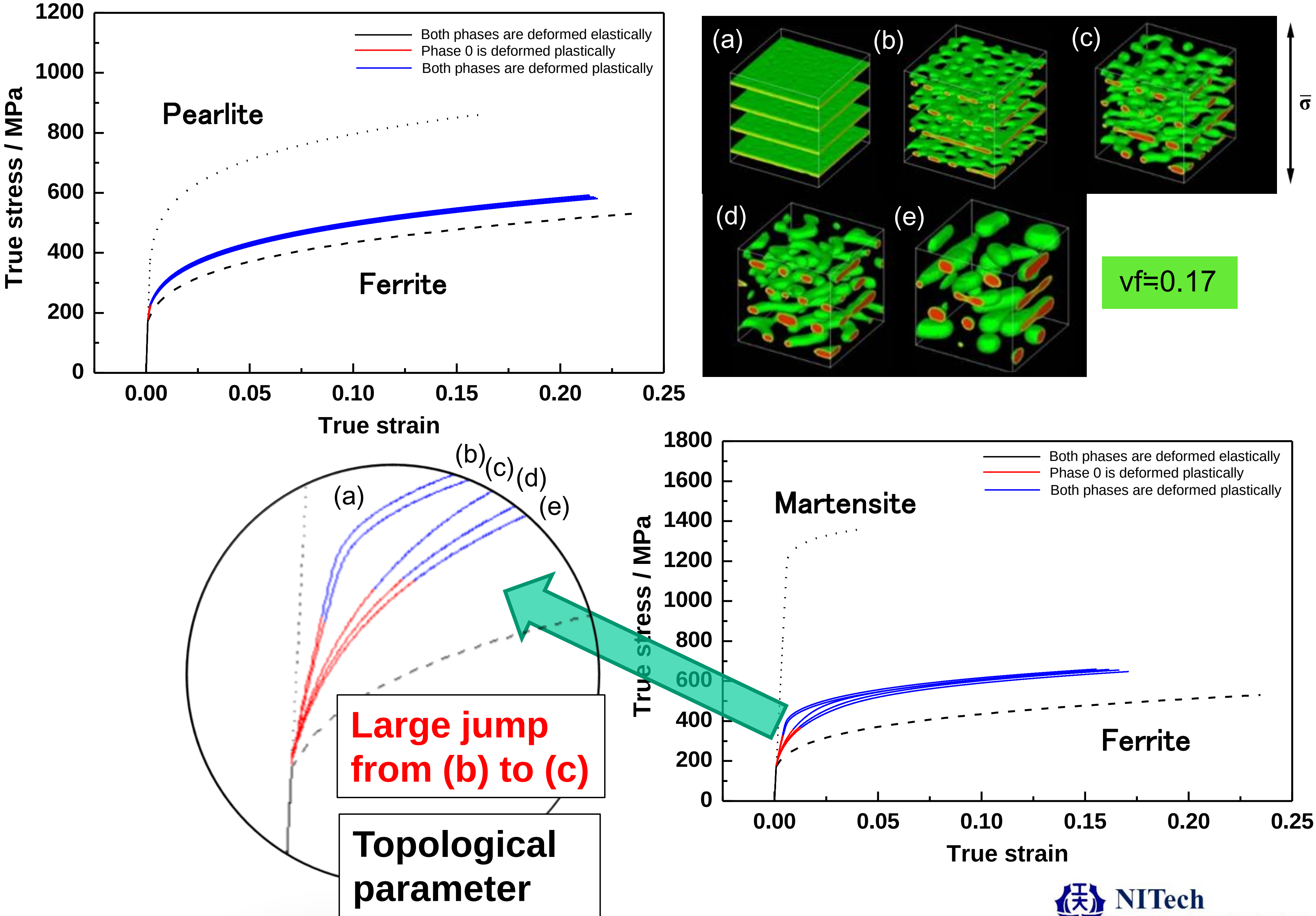

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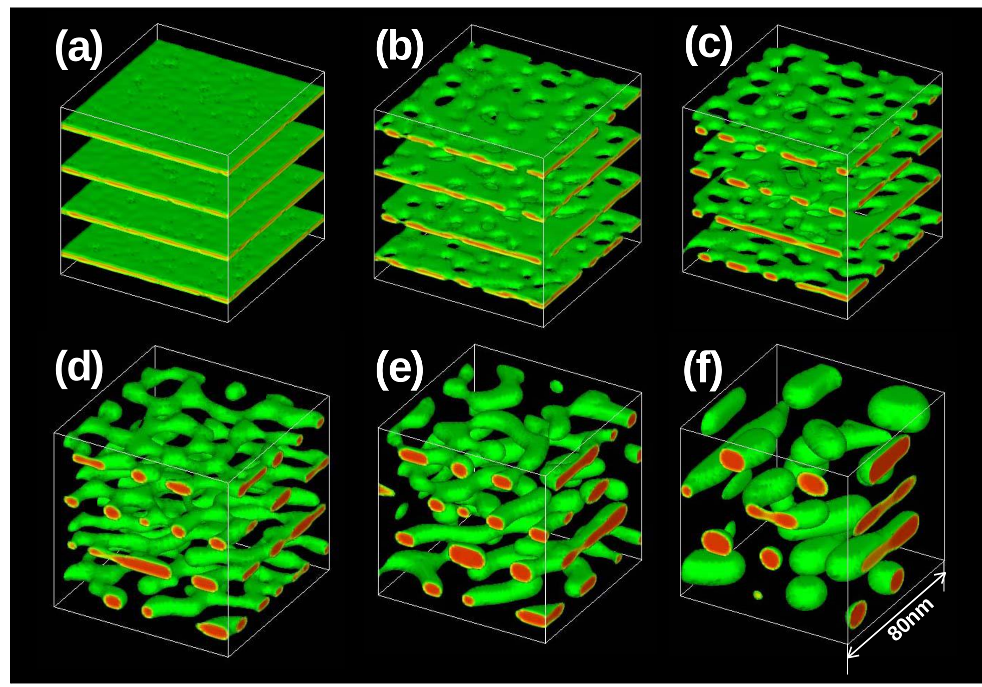
Topological parameters on 3D microstructure analysis

- **Euler characteristic:** $\chi = v - e + f = 2 - 2g,$

- **Genus:** $$g = 1 - \frac{1}{4\pi}\iint_S K d\mu,$$

$g = 1$ $g = 2$ $g = 3$

- **Connectivity:** $C = 2g,$



K **: Gaussian curvature**

H **: Mean curvature**

g: Number of holes (matrix phase) pass through the second phase

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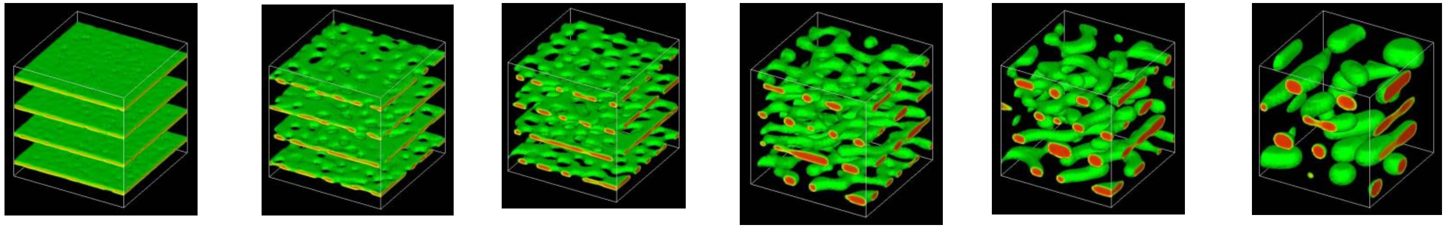
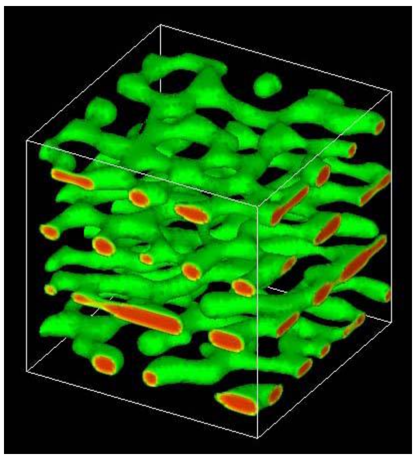
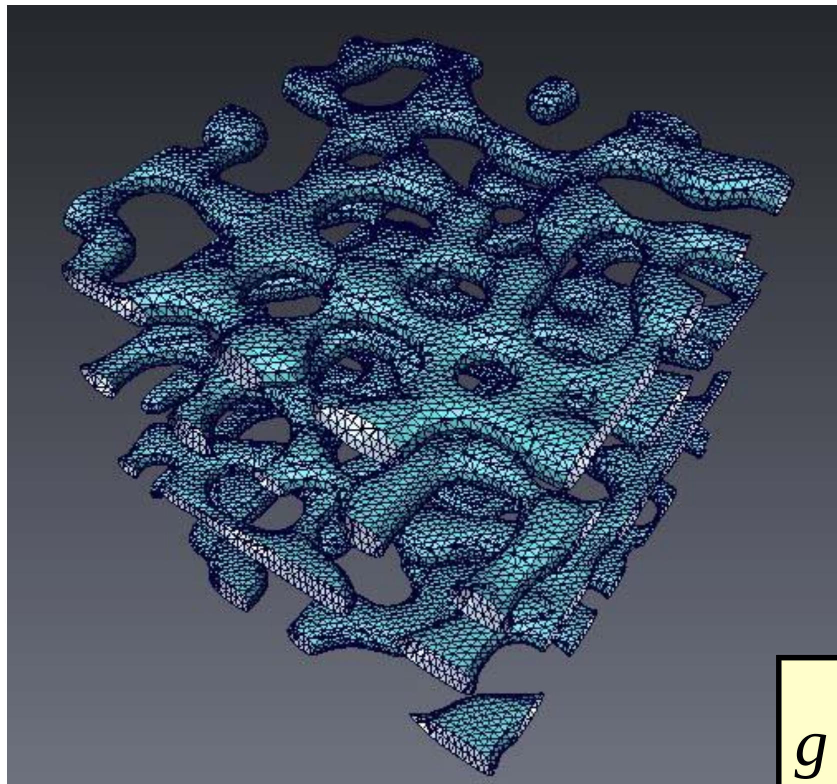
Numerical calculation method of genus



① **Iso-composition surface**



② **Triangular mesh image (STL format)**



STL file：MAVS12
Gaussian curvature：Avizo6.1

③ ***K*** **on each triangle**

④ **Integration of Gaussian curvature**

$$\iint_S K d\mu$$

⑤ **Genus:**

$$g = 1 - \frac{1}{4\pi}\iint_S K d\mu$$

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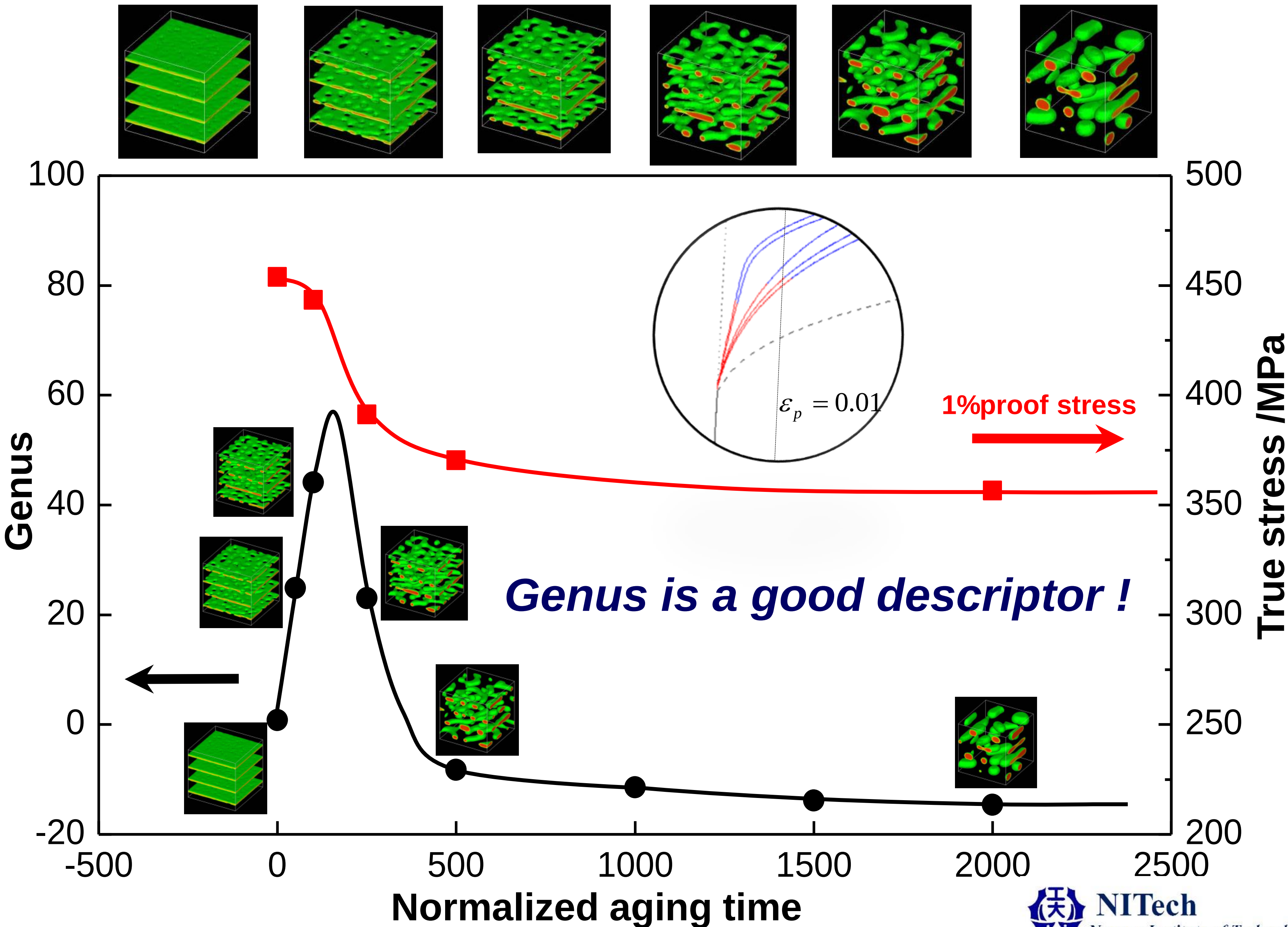
Relation between genus and 1% proof stress



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Summary

1. When the plastic deformation is dominant in both phases, the shape of S-S curve is determined only by the volume fraction of 2nd phase. Therefore, the single sphere inclusion approximation is a sufficient model to calculate S-S curve.

2. If the contribution of the elastic deformation of the 2nd phase is large, the shape of S-S curve depends not only on the volume fraction of 2nd phase but also on the morphology of microstructure.

3. As a descriptor for the mechanical property, the topological parameter Genus is a good candidate for evaluating a S-S curve of dual phase steels.

4. Since each S-S curve is calculated within few minutes on PC, the modified secant method is useful for judging whether the microstructure is important or not on the S-S curve.