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Theory of lattice strain in a material undergoing plastic deformation: Basic formulation and applications to a cubic crystal

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Theory of lattice strain in a polycrystalline aggregate under deviatoric stress is extended to include the influence of ongoing plastic deformation. When deviatoric stress is applied to a polycrystalline material at high temperatures (or above the yield stress), applied macroscopic stress is redistributed to individual grains by plastic deformation according to their orientations with respect to the macroscopic stress and plastic anisotropy of a given crystal. This microstress causes elastic deformation of individual grains that can be measured by x-ray diffraction. Consequently, the observed lattice strain depends on two material properties, viscosity (plasticity) and elastic compliance as well as the applied macroscopic stress and the stress-strain distribution among various grains. The influence of plastic deformation on lattice strain is analyzed using an anisotropic and nonlinear power-law constitutive relationship. In this model, the dependence of inferred macroscopic stress on the crystallographic orientation of diffraction plane (*hkl*) comes from elastic and plastic anisotropy of a crystal. In many materials, plastic anisotropy dominates over elastic anisotropy. This explains the observed large dependence of inferred stress on the diffraction plane and means that the determination of elastic anisotropy is difficult when plastic deformation occurs with anisotropic plasticity. When elastic anisotropy is known, plastic anisotropy of single crystal and/or stress-strain distribution in a deformed polycrystal can be determined from radial x-ray diffraction using the present model. Some examples are presented using the data on MgO.

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I. INTRODUCTION

X-ray diffraction from a polycrystalline sample at various orientations, called radial x-ray diffraction, contains rich information as to the orientation-dependent properties of constituent crystals and/or the stress acting on the bulk of the sample. This technique is particularly useful under high-pressure conditions where it is difficult to study mechanical properties using other techniques. Consequently, radial x-ray diffraction technique has been applied to study plastic properties[1–5] or elastic properties[6,7] under high-pressure conditions. However, underlying physical principles to interpret such data have not been clearly formulated and several problems have been recognized in the application of this technique. For example, the results by Mao *et al.*[6] showed vastly different elastic anisotropy of *hcp* iron calculated from the results of first-principles studies.[8–10] Also in many cases the magnitude of dependence of inferred stress on the lattice plane (*hkl*) far exceeds the values expected from Singh's model,[3,4] and the estimate of macroscopic strength of a sample from these data contains large uncertainties.

When a polycrystalline material is placed under a nonhydrostatic macroscopic stress, nonhydrostatic stress develops at each grain, leading to the elastic distortion of lattice spacings that depends on the applied stress and elastic compliance. Singh[11] developed a model of lattice strain in a polycrystalline aggregate caused by an applied macroscopic stress. This model has been used to infer either macroscopic stress and hence plastic properties or elastic constants from x-ray diffraction. However, recent studies have revealed some fundamental issues in such an exercise. The estimate of elastic anisotropy from such a method contains a systematic bias when a large plastic deformation occurs.[12]

These observations suggest that some important physics is missing in the model by Singh[11] and Uchida *et al.*[13] When a polycrystalline material is under a nonhydrostatic macroscopic stress, then nonhydrostatic stress develops at each grain (I call it *microscopic stress*) that deforms individual grain. Deformation of each grain occurs both elastically and plastically but x-ray diffraction captures only elastic part through the change in the distance between lattice planes. The stress acting on each grain (microscopic stress) causes the strain in individual grains (*microscopic strain*) and its magnitude depends on the elastic constants and the microscopic stress. When elastic constants are known then the microscopic stress can be calculated from the measured lattice strain (or vice versa). However, in order to calculate the *macroscopic stress* from microscopic stress, one needs also to know the relationship between macroscopic stress and microscopic stress.

As will be shown in the following, the model by Singh[11] is incomplete in that his model does not fully take into account the role of plastic deformation to distribute the stress acting on individual grains. Consequently, the conversion factor to translate lattice strain to macroscopic stress involves only elastic compliance tensor and hence, in this model, the variation in inferred stress with the lattice plane (i.e., $\frac{\Delta d}{d}$) is controlled only by the anisotropy of elastic compliance. When the influence of plastic deformation is included, the conversion factor includes not only the elastic compliance tensor but also the viscosity tensor. Plastic anisotropy is usually larger than elastic anisotropy and consequently the variation in inferred stress with the lattice plane [i.e., (*hkl*)] can be larger if the influence of plastic deformation is important.

Therefore, the influence of plastic deformation needs to be included in the analysis of experimental data of radial x-ray diffraction. However, previous studies to incorporate the influence of plastic deformation are all through numerical modeling using some form of self-consistent model.[3,4,14,15] In addition to the fundamental limitations of self-consistent model to explain deformation of a polycrystal with large contrast in mechanical properties (e.g., Milton[16]), it is not easy to obtain physical essence by numerical modeling. In addition, in many cases of such modeling, plastic properties are parametrized in terms of *yield stress* (*critical resolved shear stress*) that is independent of strain rate. Such a description is valid only for low-temperature plasticity but not for high-temperature plasticity. The purpose of this paper is to formulate a theory of lattice strain in a polycrystalline aggregate caused by the applied macroscopic stress including the role of plastic deformation using a power-law rheology that is appropriate for high-temperature behavior. This theory not only explains the observed large variation in inferred stress with the diffraction plane (*hkl*) but also provides a way to constrain *plastic anisotropy* of individual crystal from observed dependence of stress with the lattice plane [i.e., (*hkl*)]. In this paper, I will present a general formulation and apply it to a simple case of cubic crystal such as MgO.

II. THEORY

In order to extract useful information from measured lattice strain, we need to understand the relationship between the lattice strain and the *macroscopic stress,* Σ_{ij}, and physical properties of a given material. The lattice strain, $\frac{\Delta d}{d}$, that one measures using radial x-ray diffraction is the elastic strain caused by the stress acting on individual grains. In order to distinguish this stress from the applied stress, I will call this as *microscopic stress,* σ_{ij}, and the applied stress as *macroscopic stress*, Σ_{ij}. Consequently, the lattice strain depends on (i) the applied (macroscopic) stress, (ii) the plastic anisotropy that controls the distribution of microscopic stress for a given macroscopic stress, and (iii) the elastic compliance of a given material.

In order to calculate the lattice strain of a given crystallographic plane (*hkl*) in a plastically deforming polycrystalline material for a given orientation of diffracted x ray, I analyze the deformation of individual grain in two steps. First, I will calculate the microscopic stress caused by macroscopically imposed stress. The microscopic stress in individual grains depends on plastic anisotropy and the stress-strain distribution. Since there is no exact solution for the stress-strain distribution in plastically deforming polycrystals,[16] I will consider two cases: homogeneous stress (Sachs model) and homogeneous strain (Taylor model). Given this microscopic stress, elastic strain in individual grains can be calculated as a function of elastic constants and the orientation of the crystal. Again, elastic deformation of a crystal embedded in a polycrystalline material depends on the stress-strain distribution. It is this elastic strain of individual grains that is measured by the x-ray diffraction but the elastic strain in the individual grains is caused by the microscopic stress that depends on the plastic anisotropy. Therefore the analysis of radial x-ray diffraction needs to include the influence of both elastic and plastic deformation.

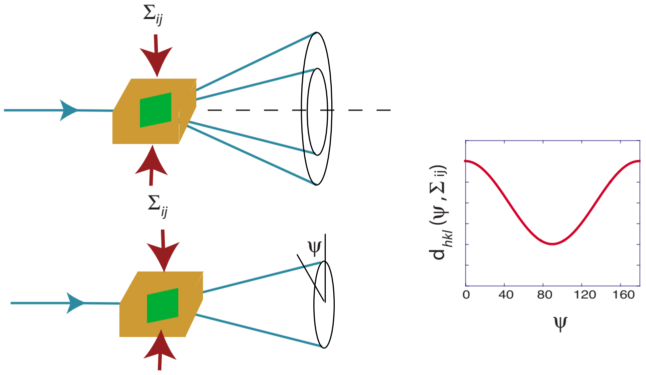

FIG. 1. (Color online) Geometry of radial x-ray diffraction. The dependence of the change in lattice spacing d_{hkl} on diffraction angle, ψ, and diffraction plane, (*hkl*), provides a useful information on macroscopic stress, Σ_{ij}, and/or other physical properties if the relation between lattice strain and these parameters is known.

Singh[11] calculated the lattice strain, $\frac{\Delta d}{d}$, for a given macroscopic stress. The x-ray diffraction by the (*hkl*) plane occurs by crystals that have orientations such that the normal to (*hkl*) is in the plane that is nearly normal to the incident x ray. If one chooses a particular 2θ for diffraction, the diffracted beam will define a cone and the diffracted beam can be captured by a detector whose position is at an angle ψ measured from some reference direction of the sample coordinate (see Fig. 1). Therefore the calculation of lattice strain involves the calculation of $\frac{\Delta d}{d}$ for a range of angle ψ corresponding to the applied macroscopic stress. The process that Singh[11] and Uchida *et al.*[13] followed is (i) to calculate the stress acting on each grain caused by the macroscopic stress from which x-ray diffraction occurs and (ii) to calculate the lattice strain for a given microscopic stress. However, the calculation of the microscopic stress caused by the macroscopic stress in Singh's model involves only the coordination transformations (from macroscopic to diffraction, and from diffraction to sample coordinate; see Fig. 2). Hence the conversion factor in his model involves only the geometrical parameters, i.e., the diffraction angle, ψ and (*hkl*). The microscopic stress (stress at each grain) for a given macroscopic stress (or strain rate) depends also on plastic anisotropy: grains with unfavorable (favorable) orientation for plastic flow will have higher (lower) stresses. Therefore, the first step in this calculation should be to calculate the microscopic stress (for a sample reference frame) corresponding to a given macroscopic stress.

In a plastically deforming material, stress at an individual grain depends on the plastic properties of that grain, the orientation of the grain with respect to the applied stress and the boundary condition. The boundary condition reflects the nature of grain-grain interaction that cannot be exactly formulated (see, e.g., Milton[16]). To simplify the calculation, I postulate that the actual (microscopic) stress is an average of stress corresponding to two end members (homogeneous stress and homogenous strain), viz.,

$$\sigma_{ij} = \alpha \cdot \sigma_{ij}^{S} + (1-\alpha) \cdot \sigma_{ij}^{T}, \tag{1}$$

where α $(1 \geq \alpha \geq 0)$ is a parameter that characterizes the stress-strain distribution for plastic deformation [$\alpha=1$ for homogeneous stress (Sachs) model, $\alpha=0$ for homogeneous strain (Taylor) model], σ_{ij}^{S} is the stress for the Sachs model

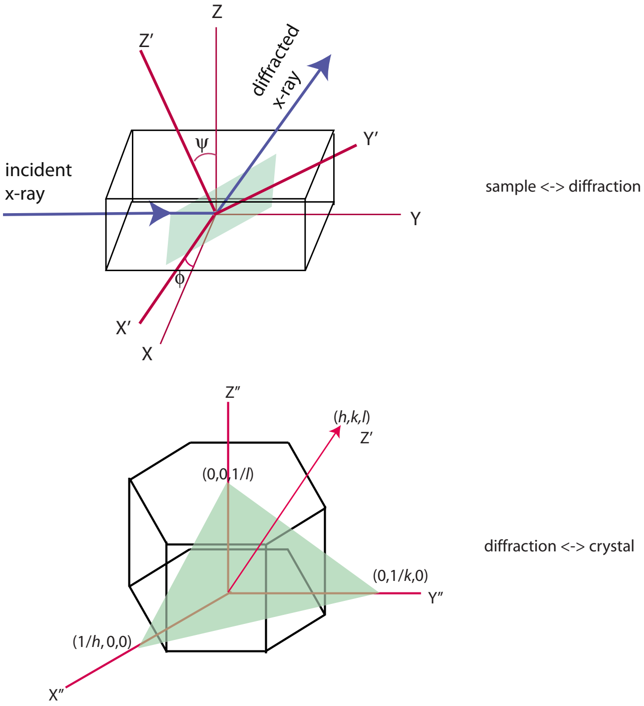

FIG. 2. (Color online) Definitions of three coordinate systems (X, Y, and Z: sample coordinates; X', Y', and Z': diffraction coordinates; and X'', Y'', and Z'': crystal coordinates) and ψ and (hkl).

($=\Sigma_{ij}$: macroscopic stress), and σ^T_{ij} is the stress corresponding to the Taylor model. Equation (1) is written in the sample reference frame. For σ^S_{ij}, the results are identical to those by Singh.

In order to treat plastic deformation, it is convenient to separate volumetric and shear stress/strain. Thus, for a volumetric component, one has

$$\sigma_P = \alpha \cdot \sigma^S_P + (1-\alpha) \cdot \sigma^T_P, \tag{2}$$

where $\sigma_P = \frac{\sigma_{11}+\sigma_{22}+\sigma_{33}}{3} (=P)$ is a compressional stress (pressure), and an equation similar to Eq. (1) is applied to shear stress. Since x-ray diffraction experiments are usually conducted for a long time compared to the time scale of microscopic relaxation processes, I consider a fully relaxed state of volumetric compression, i.e., $\alpha=1$, then Eq. (2) is reduced to the isothermal equation of state, viz.,

$$P = P\left(T, \frac{\Delta V}{V}\right), \tag{3}$$

where T is the temperature and $\frac{\Delta V}{V} = \varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}$ is the volumetric strain. This relation can be used to determine the pressure when temperature is known. In the following, I will focus on deviatoric strain and associated deviatoric stress.

The deviatoric (shear) stress is related to deviatoric (shear) strain or deviatoric (shear) strain rate. When large plastic deformation occurs, then the distribution of shear stress is determined mostly by viscous flow, viz.,

$$\sigma^T_{ij} = 2\eta_{ijpq}\dot{E}_{pq}, \tag{4a}$$

where $\dot{E}_{pq}$ is the macroscopically imposed strain rate and η_{ijpq} is the viscosity tensor (in the sample coordinate) that depends on the plastic properties of the crystal and the orientation of the crystal with respect to the applied stress. Plastic deformation of a material often follows nonlinear relation between the applied stress and strain rate called power-law creep.[17,18] The viscosity tensor for a material deformed by the power-law creep may be written as (Appendix)

$$\sigma^T_{ij} = 2\bar{\eta}_{ijpq} II_{\dot{E}}^{1-n/2n}\dot{E}_{pq}, \tag{4b}$$

where n is the stress exponent, $\bar{\eta}_{ijpq}$ is the (microscopic) viscosity coefficient tensor for nonlinear rheology (unit is Pa s$^{1/n}$) that depends on the strain rate, and $II_{\dot{E}}$ is the second invariant of the strain-rate tensor. The macroscopic strain rate, $\dot{E}_{pq}$, and its second invariant, $II_{\dot{E}}$, are known for a particular experimental setup.

Equations (4a) and (4b) may be cast into a matrix form using the Voigt notation (e.g., Nye[19]), viz.,

$$\sigma^T_i = 2\eta_{ij}\dot{E}_j \quad (\text{Voigt notation}), \tag{5a}$$

and

$$\sigma^T_i = 2\bar{\eta}_{ij} II_{\dot{E}}^{1-n/2n}\dot{E}_j \quad (\text{Voigt notation}), \tag{5b}$$

respectively.

Similarly, the macroscopic strain rate, $\dot{E}_j$, is related to the macroscopic stress, Σ_i, as

$$\Sigma_i = 2\bar{H}_{ij} II_{\dot{E}}^{1-n/2n}\dot{E}_j \quad (\text{Voigt notation}), \tag{6}$$

where $\bar{H}_{ij}$ is the macroscopic viscosity coefficient. Inserting Eq. (6) into Eq. (4), I obtain

$$\sigma^T_i = \bar{\eta}_{ik}\bar{H}^{-1}_{kj}\Sigma_j \equiv \xi_{ij}\Sigma_j \quad (\text{Voigt notation}), \tag{7}$$

with

$$\xi_{ij} \equiv \bar{\eta}_{ik}\bar{H}^{-1}_{kj} \quad (\text{Voigt notation}), \tag{8}$$

where $\bar{H}^{-1}_{kj}$ is the inverse of the macroscopic viscosity coefficient matrix, $\bar{H}_{kj}$. Relation (7) relates the macroscopic stress to the microscopic stress in the homogeneous strain model (Taylor model). This relation indicates that the microscopic stress depends on microscopic ($\bar{\eta}_{ij}$) and macroscopic ($\bar{H}_{ij}$) plastic anisotropy. Macroscopic plastic anisotropy is due to the lattice-preferred orientation (LPO) and the plastic anisotropy of individual crystals, and therefore anisotropy of $\bar{H}_{ij}$ is always weaker than that in $\bar{\eta}_{ij}$. In a case where macroscopic anisotropy is much smaller than anisotropy of a crystal (weak LPO), Eq. (7) becomes

$$\sigma^T_{ij} \approx \frac{\bar{\eta}_{ijpq}}{\langle \bar{H} \rangle}\Sigma_{pq}, \tag{9}$$

where $\langle \bar{H} \rangle$ is the isotropic macroscopic viscosity coefficient of the sample.

Inserting Eq. (7) into Eq. (1), I have

$$\sigma_{ij} = \alpha \cdot \Sigma_{ij} + (1-\alpha) \cdot \xi_{ijpq}\Sigma_{pq}. \tag{10a}$$

In order to calculate lattice strain, it is useful to rewrite Eq. (10a) in terms of the crystal coordinate, viz.,

$$\sigma''_{ij} = \alpha \cdot \Sigma''_{ij} + (1-\alpha) \cdot \xi''_{ijpq}\Sigma''_{pq}, \tag{10b}$$

where $''$ indicates that the quantity is written using the crystal coordinate, quantities without any prime means that it is written using the sample coordinate (for the definitions of various coordinates see Fig. 2).

Stress in this equation may be transformed to the stress in the sample coordinate using the procedure described by Singh[11] and Uchida *et al.*,[13] viz.,

$$\Sigma''_{ij} = c_{ip} \cdot c_{jq} \cdot \Sigma_{pq}, \tag{11}$$

where

$$c_{ij} = a_{ik}b_{kj}, \tag{12}$$

with

$$a_{ij} = \begin{bmatrix} \cos\varphi & -\sin\varphi\cos\psi & \sin\varphi\sin\psi \\ \sin\varphi & \cos\varphi\cos\psi & -\cos\varphi\sin\psi \\ 0 & \sin\psi & \cos\psi \end{bmatrix}, \tag{13}$$

where (φ,ψ) is defined in Fig. 2 and

$$b_{ij} = \begin{bmatrix} \dfrac{N}{M} & 0 & \dfrac{h}{M} \\ -\dfrac{hk}{NM} & \dfrac{l}{N} & \dfrac{k}{M} \\ -\dfrac{hl}{NM} & -\dfrac{k}{M} & \dfrac{l}{M} \end{bmatrix}, \tag{14}$$

with $N \equiv \sqrt{k^2+l^2}$, $M \equiv \sqrt{h^2+k^2+l^2}$.

After transformation, the microscopic stress is expressed in terms of the macroscopic stress (Σ_{ij}), viscosity coefficient tensor of a crystal $(\bar{\eta}''_{ijpq})$, viscosity coefficient tensor of a sample $(\bar{H}_{ijpq})$, and the index of lattice plane from which diffraction occurs $[(hkl)]$ and the orientation of that plane with respect to the x-ray detector (ψ). Therefore in general, one obtains a functional relationship between microstress and these variables as

$$\sigma''_{ij} = \sigma''_{ij}(\psi, hkl \| \bar{\eta}''_{ijpq}, \bar{H}_{ijpq}; \Sigma_{ij}; \alpha). \tag{15}$$

Given the expression for stress in the crystal coordinate, σ''_{ij}, one can calculate the strain in each crystal in a polycrystal. Strain in a crystal embedded in a polycrystalline material depends on the stress-strain distribution for elastic deformation and I use a simple formula,[11,13]

$$\varepsilon''_{ij} = \beta \cdot \varepsilon''^{R}_{ij} + (1-\beta) \cdot \varepsilon''^{V}_{ij}, \tag{16}$$

where β represents the stress-strain distribution for elastic deformation (β=1 for homogeneous stress, β=0 for homogeneous strain), ε''^{R}_{ij} is the strain for homogeneous stress (Reuss model), and ε''^{V}_{ij} is the strain for homogeneous strain (Voigt model). As far as the stress is small, linear elasticity works and hence,

$$\varepsilon''^{R,V}_{ij} = S''^{R,V}_{ijpq}\sigma''_{pq}, \tag{17}$$

where $S''^{R,V}_{ijpq}$ is the elastic compliance for the Reuss or Voigt state (in the crystal coordinate). Given ε''_{ij}, we can calculate the lattice strain, ε'_{hkl} (strain normal to the diffraction plane), by ($'$ indicates that the quantity is written in terms of the diffraction coordinate)

$$\varepsilon'_{hkl} = \varepsilon'_3 = \varepsilon''_{ij}l_i l_j = \left(\frac{\Delta d}{d}\right)^{hkl}, \tag{18}$$

where l_i is the direction cosine between x'_3 and x''_i. Note that stress-strain distribution for elastic deformation can be different from that for plastic deformation, and therefore the values of α and β can also be different. I finally obtain

$$\left(\frac{\Delta d}{d}\right)^{hkl} = G(\psi, hkl \| \Sigma_{ij}; S''_{ijpq}, \bar{\eta}''_{ijpq}, \bar{H}_{ijpq}; \alpha, \beta), \tag{19a}$$

where $G(\psi, hkl \| \Sigma_{ij}; S''_{ijpq}, \bar{\eta}''_{ijpq}, \bar{H}_{ijpq}; \alpha, \beta)$ is a function of known variables, (ψ, hkl), and unknown variables, $(\Sigma_{ij}; S''_{ijpq}, \bar{\eta}''_{ijpq}, \bar{H}_{ijpq}; \alpha, \beta)$, where S''_{ijpq} and $\bar{\eta}''_{ijpq}$ are the properties of the crystal (elastic compliance and viscosity coefficient). Macroscopic viscosity coefficient tensor, $\bar{H}_{ijpq}$, depends on the anisotropy of crystal plasticity and the LPO; the latter may be determined from x-ray intensity or from the orientation measurements of crystals in a sample. For simplicity, I will consider a case of weak LPO and the influence of LPO will not be included in the following analysis. In such a case, Eq. (19a) is reduced to

$$\left(\frac{\Delta d}{d}\right)^{hkl} = G\left(\psi, hkl \| \Sigma_{ij}; S''_{ijpq}, \frac{\bar{\eta}''_{ijpq}}{\langle \bar{H} \rangle}; \alpha, \beta\right). \tag{19b}$$

Equation (19b) contains three types of variables: the angle, ψ, at which diffracted x ray is detected, the macroscopic stress (Σ_{ij}), anisotropic physical properties $(S''_{ijpq}, \frac{\bar{\eta}''_{ijpq}}{\langle \bar{H} \rangle})$, and the parameters that characterize the stress-strain distribution (α, β). X-ray diffraction measurements are made for a finite number of independent (hkl) planes. Diffracted x-ray beams are collected somewhat differently between white x-ray and monochromatic x-ray diffraction: for a white x-ray, one uses fixed finite values of ψ, whereas for a monochromatic x-ray, one uses continuous values of ψ. However in both cases, the number of independent information from the ψ dependence is finite because Eq. (19) contains only a finite number of $(\sin\psi, \cos\psi)$.

It is seen from Eq. (19b) that the radial x-ray diffraction data depend on various parameters and therefore in order to obtain one (or a few) unknown parameter(s) one needs to know other parameters. For example, in general the lattice strain is proportional to stress, elastic compliance, and viscosity coefficient, $(\frac{\Delta d}{d})^{hkl} \propto (\Sigma_{ij}) \cdot (S''_{ijpq}) \cdot (\frac{\bar{\eta}''_{ijpq}}{\langle \bar{H} \rangle})$, and hence, one needs to know both elastic compliance and viscosity anisotropy in order to determine the stress. As will be shown below, in some cases, these unknowns including (α, β) can be determined separately using the fact that the dependence of these unknowns on $(\psi; hkl)$ is different.

Let us consider a case where elastic anisotropy is much weaker than plastic anisotropy. This is a case for most materials where plastic anisotropy is much stronger than elastic anisotropy when plastic deformation occurs by dislocation motion.[20] In such a case, the difference between Voigt and Reuss models is small compared to plastic anisotropy, and I will use the Voigt model for elastic deformation, viz.,

$$\varepsilon''_{ij} = \varepsilon''^{V}_{ij} = S^{V}_{ijpq}\sigma''_{pq}, \tag{20}$$

where S^{V}_{ijpq} is the elastic compliance for the Voigt average (β=0) that is independent of (ψ,hkl). In this case, the dependence of lattice strain on (hkl) is only through the dependence of microscopic stress on (hkl). Under this assumption, only unknowns are the viscous anisotropy ($\bar{\eta}''_{ijpq}$), the macroscopic stress (Σ_{ij}) and α, and a parameter to characterize the stress-strain distribution in a plastically deforming aggregate.

III. APPLICATIONS TO TRIAXIAL COMPRESION OF AN AGGREGATE OF CUBIC CRYSTALS

In order to illustrate how the present theory is used to analyze the data on radial x-ray diffraction, let us consider a simple case: deformation of a polycrystalline aggregate made of a cubic crystal deformed by triaxial compression. In this case, there are only two independent viscosities (Appendix), and there is only one deviatoric stress component. Consequently, Eq. (19) can be written in a compact form. Let us consider, for simplicity, a case where elastic anisotropy is much smaller than plastic anisotropy and the influence of LPO is negligible. Under these conditions, the lattice strain caused by the macroscopic stress essentially depends on plastic and elastic anisotropy with the assumption of β=0. Relation (19b) is then written as

$$\frac{\Delta d}{d} = \alpha \cdot \left(\frac{\Delta d}{d}\right)^{S} + (1-\alpha)\cdot\left(\frac{\Delta d}{d}\right)^{T}, \tag{21}$$

with

$$\begin{aligned}\left(\frac{\Delta d}{d}\right)^{T} &= t\cdot f(\psi)\cdot S''_{44}\cdot \eta^{*}_{I}\cdot\left[\Gamma(hkl)\cdot(A-B)-\frac{A}{3}\right]\\ &= t\cdot f(\psi)\cdot S''_{44}\cdot\left[\Gamma(hkl)\cdot(A\cdot\eta^{*}_{I}-\eta^{*}_{II})-\frac{A}{3}\eta^{*}_{I}\right],\end{aligned} \tag{22a}$$

and

$$\left(\frac{\Delta d}{d}\right)^{S} = t\cdot f(\psi)\cdot S''_{44}\cdot\left[\Gamma(hkl)\cdot(A-1)-\frac{A}{3}\right], \tag{22b}$$

where $t=\Sigma_3-\Sigma_1$, $f(\psi)=1-3\cos^2\psi$, $A=\frac{2(S''_{11}-S''_{12})}{S''_{44}}$, $B=\frac{\bar{\eta}''_{II}}{\bar{\eta}''_{I}}$, $\Gamma(hkl)=\frac{h^2k^2+k^2l^2+h^2l^2}{(h^2+k^2+l^2)^2}$, and $\eta^{*}_{I,II}=\frac{\bar{\eta}''_{I,II}}{\langle\bar{H}\rangle}$. The parameter A represents the elastic anisotropy and the parameter B represents the plastic anisotropy. Therefore

$$\frac{\Delta d}{d} = t\cdot f(\psi)\cdot S''_{44}\cdot[C_1\cdot\Gamma(hkl)+C_2], \tag{23a}$$

with

$$C_1 = (A\,\eta^{*}_{I}-\eta^{*}_{II}) + \alpha[A(1-\eta^{*}_{I})-(1-\eta^{*}_{II})], \tag{23b}$$

and

$$C_2 = -\frac{A}{3}[\eta^{*}_{I}+\alpha(1-\eta^{*}_{I})]. \tag{23c}$$

These relations form the basis for interpreting the results of radial x-ray diffraction in terms of physical properties of a material. The procedure of interpreting experimental data may be as follows. First, for each diffraction planes, (hkl), lattice strain should be measured as a function of orientation of diffracted x ray (ψ) in order to separate the volumetric and deviatoric strain components. The volumetric component of strain is used to determine the pressure (for a given temperature), and the deviatoric component is used to determine the deviatoric stress and plastic properties. For triaxial compression, one needs at least two angles to determine the deviatoric strain, say ψ=0 and $\frac{\pi}{2}$.

Second, the relation between deviatoric lattice strain and the index of diffraction plane, (hkl), can be used to determine various unknown parameters. Because the influence of diffraction plane on lattice strain, $\frac{\Delta d}{d}$, is expressed by a singe term, $\Gamma(hkl)$, by a linear equation [Eq. (23a)], one can determine only two parameters from the observed deviatoric lattice strain. In a case where all the material properties (i.e., elastic, compliance, and viscosity coefficients) are known, then Eqs. (23a)–(23c) can be used to determine the macroscopic stress, t (i.e., macroscopic viscosity coefficient), and a parameter, α, much the same way as Funamori *et al.*[1] In other words, when microscopic viscosity coefficients are known, relation (23) can be used to determine the macroscopic viscosity coefficient and the stress-strain distribution in an aggregate.

However, in many cases plastic properties of the constituent crystal are unknown. In these cases, the relation [Eqs. (23a)–(23c)] cannot be used to determine unknowns uniquely because there are only two equations for four unknowns (t, α, η^{*}_{I}, and η^{*}_{II}). However, some general conclusions can be derived from Eqs. (23a)–(23c). For example, the lattice strain ratio for (hkl)=(111) and (200) is given by

$$\frac{X(111)}{X(200)} = \frac{1}{A}\frac{\eta^{*}_{II}+\alpha(1-\eta^{*}_{II})}{\eta^{*}_{I}+\alpha(1-\eta^{*}_{I})}, \tag{24}$$

where $X(hkl)$ is the deviatoric lattice strain for the diffraction plane (hkl) defined by Eq. (23a). If stress distribution is homogeneous, i.e., α=1, then, $\frac{X(111)}{X(200)}=\frac{1}{A}\approx 0.8$. This is much smaller than the observed value for MgO (at high stress).[3,21] Therefore I conclude that the stress distribution in deformed MgO is highly heterogeneous under these experimental conditions. Another extreme case is the homogeneous strain, i.e., α=0. In this case, $A\frac{X(111)}{X(200)}=\frac{\eta^{*}_{II}}{\eta^{*}_{I}}$ so that one can determine $B(=\frac{\eta^{*}_{II}}{\eta^{*}_{I}})$, from observed ξ using $\xi=B$.

In a general case of intermediate stress-strain distribution ($1\geq\alpha\geq 0$), one has four unknowns (t, α, η^{*}_{I}, and η^{*}_{II}), but Eqs. (23b) and (23c) provide only two constraints, viz.,

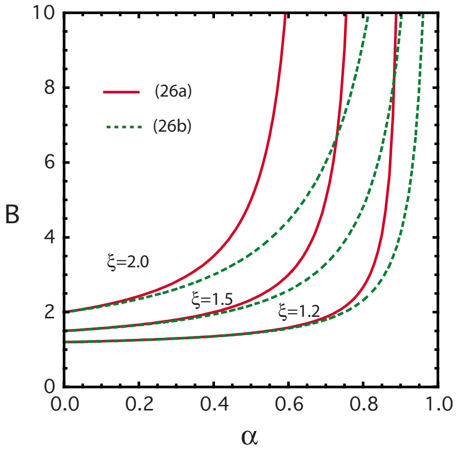

FIG. 3. (Color online) The relation between a parameter characterizing stress-strain distribution (α) and plastic anisotropy [$B(=\frac{\eta^*_{II}}{\eta^*_I})$] for various values of $\xi(=A\cdot\frac{X(111)}{X(200)})$ and the relation for microscopic and macroscopic viscosity [Eq. (26a) or Eq. (26b)].

$$X(111) = -\frac{1}{3}t\cdot S''_{44}\cdot[\eta^*_{II}+\alpha(1-\eta^*_{II})]. \tag{25a}$$

$$X(200) = -\frac{1}{3}t\cdot S''_{44}\cdot A\cdot[\eta^*_{I}+\alpha(1-\eta^*_{I})]. \tag{25b}$$

An additional relation is a relation between macroscopic viscosity and microscopic viscosity such as

$$\frac{\eta^*_I+\eta^*_{II}}{2} = 1, \tag{26a}$$

or

$$\frac{(\eta^*_I)^{-1}+(\eta^*_{II})^{-1}}{2} = 1. \tag{26b}$$

Relation (26a) corresponds to homogeneous strain, whereas relation (26b) corresponds to homogeneous stress.

When Eq. (26a) or Eq. (26b) is assumed, then we have three relations and therefore, if one assumes α, one can determine all other unknowns. To illustrate this procedure, I have calculated $B(=\frac{\eta^*_{II}}{\eta^*_I})$ for various values of α and $\xi(=A\cdot\frac{X(111)}{X(200)})$. The results are shown in Fig. 3. Given $B(=\frac{\eta^*_{II}}{\eta^*_I})$, one can then calculate η^*_I and η^*_{II} using the relation (26a) or Eq. (26b). Then the macroscopic stress (i.e., macroscopic viscosity) can be calculated using the relation (25a) or Eq. (25b). The relations between $B(=\frac{\eta^*_{II}}{\eta^*_I})$ and $\xi(=A\cdot\frac{X(111)}{X(200)})$ using relation (26a) are valid for homogeneous strain (i.e., small α) and those using the relation in Eq. (26b) are valid for homogeneous stress (i.e., large α). However, Fig. 3 shows that the choice of relation (26a) or Eq. (26b) has only a small effect on the calculated value of plastic anisotropy, B. Therefore a more realistic case will be well bounded by these two end-member cases. In both cases the plastic anisotropy, B, corresponding to a given ξ is relatively insensitive to α as far as α is small (<0.5) when ξ is not very large. However, when α is large, then B is highly sensitive to α. This means that when the stress-strain distribution is close to homogeneous strain (small α), then the parameter α cannot be determined precisely but the parameter B (plastic anisotropy) is well constrained. The opposite is true when α is large, i.e., a case for nearly homogeneous stress. It is noted that an ambiguity of a parameter α can be eliminated or reduced if the stress/strain distribution of individual grains in a deformed sample is measured.[22,23]

Let us compare the present theory with some experimental observations on MgO based on radial x-ray diffraction. The best results to compare with the present theory are those by Mei *et al.*[24] where deformation experiments were made at T (temperature)$=1373-1573$ K at P (pressure)$=1.5-10$ GPa under which conditions deformation likely occurs by the power-law dislocation creep.[25] Mei *et al.*[24] reported $\xi(=A\cdot\frac{X(111)}{X(200)})\sim 2.2$ at $T=1373$ K and $P=2.4-3.1$ GPa, ~ 2.0 at $T=1373$ K and $P=8.8$ GPa, ~ 2.0 at $T=1473$ K and $P=4.4$ GPa, and ~ 1.85 at $T=1573$ K and $P=1.5-4.0$ GPa. In other words, $\xi>1$ and ξ decreases with (homologous) temperature. $\xi(=A\cdot\frac{X(111)}{X(200)})>1$ means $B(=\frac{\eta^*_{II}}{\eta^*_I})>1$, and the latter is consistent with the known property of MgO.[26,27] Although some results are available at lower temperatures,[2,3] the results at lower temperatures are difficult to interpret because of the large influence of work hardening.[2] However, the general trend is similar, i.e., $\xi(=A\cdot\frac{X(111)}{X(200)})>1$, which can be interpreted by the plastic anisotropy. In order to make a quantitative analysis, I chose the results for experiments in which boron epoxy was used as a pressure medium. Using their data, I calculated ξ and compared these results with plastic anisotropy factor, B (the parameter B is calculated from the experimental data by Copley and Pask[26]). The influence of pressure is included assuming that the temperature dependence of plastic anisotropy follows the homologous temperature scaling, i.e., $B\propto\exp\left(\gamma\frac{T_m(P)}{T}\right)$where γ is a constant and $T_m(P)$ is melting temperature. I used melting temperature data from Zerr and Boehler.[28] Figure 4(a) shows the results. B and ξ correlate well suggesting that the observed (hkl) dependence of stress, ξ, is largely due to the plastic anisotropy of single crystals. However, the values of B are systematically larger than those of ξ. Using the results shown in Figs. 3 and 4(a), I calculated a parameter α and plotted it as a function of temperature. Figure 4(b) shows that α increases with temperature; i.e., stress becomes more homogeneous at higher temperatures.

IV. DISCUSSIONS

In his classical paper on the radial x-ray diffraction, Singh[11] did mention plastic deformation (p. 4279). However, the most important role of plastic deformation, i.e., the distribution of stress among individual grains was not included in his model. Instead, Singh considered that stress causes plastic deformation but it was assumed that at a certain point a sample achieves mechanical *equilibrium* implying no

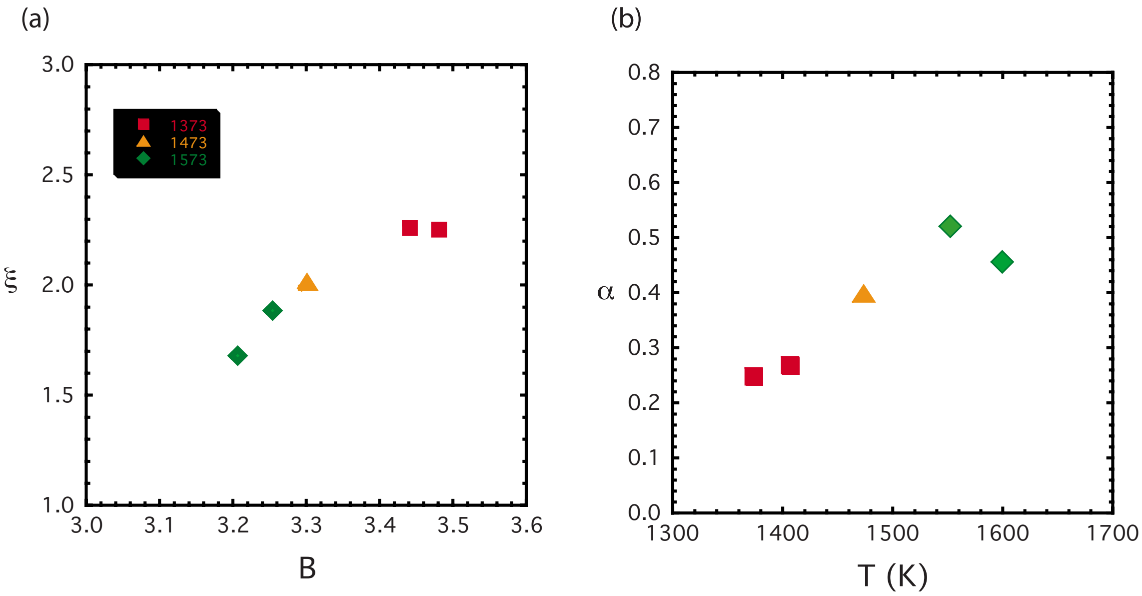

FIG. 4. (Color online) (a) A comparison of plastic anisotropy, B, with the observed values of (hkl) dependence of stress, ξ. (b) Parameter α calculated from the observed values of ξ using the relation shown in Figs. 3 and 4(a) as a function of temperature (temperature for each data is normalized to $P=2.4$ GPa) using the homologous temperature scaling.

continuing plastic deformation. Consequently, he considered that the influence of plastic deformation can be included if one allows a range of stress-strain distribution in elastically deformed material. In other words, the macroscopic strain rate is assumed to be zero, $\dot{E}_{ij}=0$. Such would be the case of a relaxed state of a Voigt model. However, under most high-temperature conditions, a given material will continue to deform under deviatoric stress ($\dot{E}_{ij}\neq 0$). Even in such a case, microscopic elastic deformation (microscopic equilibrium) also occurs in the constituent crystals. Such a model is called a Maxwell model. The model considered in the present paper corresponds to a Maxwell model.

Another limitation in a conventional approach[3,11,14,15] is that plastic deformation is considered to provide *yielding* and the differential stress is interpreted as a *yield stress* (or *critical resolved shear stress*) that is independent of strain rate. *Critical resolved stress* used in many self-consistent models belongs to this category of description of plastic deformation.[17] However, under most high-temperature conditions, the concept of yield stress (or critical resolved stress) is not appropriate and the strength depends strongly on strain rate. The power-law constitutive relationship used in this paper is a more appropriate form of constitutive equation under these conditions. In these cases, a sample is not in the mechanical equilibrium at the macroscopic scale, yet a sample can achieve elastic equilibrium at the scale of individual grains. X-ray diffraction captures this microscopic elastic equilibrium.

A so-called self-consistent approach used to interpret the results of radial x-ray diffraction[3,14] assumes some type of interaction among grains. This is equivalent to an assumption of a particular value of α in my model. However, the choice of this parameter is implicit in the self-consistent approach and the validity of such a choice is not known. Also a self-consistent approach does not explain a behavior of aggregates when strength contrast is large.[17,22]

The above theory is quite general, but replies on some assumptions. First, when deformation occurs at low temperatures and/or low stresses, then plastic deformation is not significant and the classical model by Singh[11] will apply. In fact, Weidner and Li[21] showed that when the applied stress is below the critical value, then the results of radial x-ray diffraction are consistent with the model by Singh.[11] The same is true when deformation occurs by diffusion creep. Diffusion in a cubic crystal is isotropic, and hence there will be no plastic anisotropy in such a case and the results of radial x-ray diffraction should agree with those of a classic theory. Second, the assumption of a linear combination of the stress corresponding to two extreme cases is a crude approximation. However, this relation allows us to infer the state of stress-strain distribution and hence the macroscopic strength of a plastically deforming material. Second, the nonlinear flow law of form (4b) is also an approximate form. The power-law constitutive relation is valid only under limited conditions (at high temperature and low stress). At low-temperature and/or high-stress conditions, another form of constitutive relation is more appropriate. Incorporation of other flow law is straightforward as far as one parameter is used to characterize the strength at a given condition. Third, the influence of LPO is not discussed in any detail. This is justified to a first-order approximation because the first-order effect of LPO is to change the intensity of x-ray diffraction but not the positions (angle or energy) of diffraction peaks. If needed, the influence of LPO may be included in two steps in this theory: one in averaging over φ,[29] and another in converting imposed macroscopic strain field to macroscopic stress field. The formula for lattice strain can be substantially simplified when the influence of LPO is weak. For more detailed discussion on the influence of LPO on lattice strain see Merkel and Yagi.[29] It is often argued that the discrepancy between the experimental[6] and theoretical results[8] on elastic anisotropy is largely due to LPO.[9,30] Although LPO has some influence on the calculated elastic anisotropy from radial x-ray diffraction, such an effect is indirect and small. The effect of plastic anisotropy is direct and in most cases much larger and more important.

The present theory provides a clear explanation of the observed results of radial x-ray diffraction at high pressures (and temperatures) that are inconsistent with a classic theory of Singh.[11] In addition, the present theory makes it possible to obtain some constraints on plastic anisotropy of single crystals or stress-strain distribution from the results of radial x-ray diffraction of polycrystalline samples. In case of MgO where some results of radial x-ray diffraction are available, I show that the observed large (*hkl*) dependence of stress can be attributed to large plastic anisotropy, and if the known plastic anisotropy is used then one can infer the variation in stress distribution with temperature. The results show that stress becomes more homogeneous as temperature increases, which is presumably due to the enhanced plastic accommodation. Such results have important bearing on the understanding of fabric (texture) development in and the strength of deformed polycrystals.[31] However, there are large uncertainties in the experimental data on radial x-ray diffraction. For example, for MgO, diffraction from (111) is weaker than that that from (200), and consequently, errors are larger for (111) than for (200). This causes some uncertainties for ξ. Mei *et al.*[24] used boron epoxy pressure medium below 4.4 GPa and mullite above 8.8 GPa. I did not compare results with different pressure media because there is a potential bias caused by the difference in pressure media through the systematic difference in water content in samples. Consequently, the pressure range explored is limited and the influence of pressure on plastic anisotropy and/or stress-strain distribution in a deformed polycrystal of MgO is not well characterized by the present study. Because the relative easiness of two slip systems in MgO (B1 structure) is due largely to the influence of electrostatic energy that changes with pressure,[32] one expects that plastic anisotropy in materials with B1 structure will change with pressure. With higher quality data coming from improved x-ray diffraction measurements, the present theory will help us understand the variation in plastic anisotropy and the stress-strain distribution with pressure (and temperature). The expansion of the present theory to more general stress geometries and/or to other crystal structures is straightforward and will be discussed in the next papers.

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APPENDIX: FORMULATION OF NONLINEAR FLOW LAW AND PLASTIC ANISOTROPY

Plastic deformation of a crystal often occurs by the motion of crystal dislocations. In most cases, the rate of deformation is a nonlinear function of stress. When the stress level is modest and temperature is a large fraction of the melting temperature ($>0.5\ T/T_m$, T_m: melting temperature), strain rate is proportional to some power of stress. Let us considera material that deforms at steady state following a power-law rheology. Because both stress and strain rate are second-rank tensors, the constitutive relation connecting them must involve a fourth-rank tensor. I choose the following formula that is a generalization of the well-known Levy–von Mises formula for anisotropic plasticity,[33]

$$\sigma_{ij} = 2\bar{\eta}_{ijpq} II_{\dot{\varepsilon}}^{1-n/2n} \dot{\varepsilon}_{pq}, \tag{A1}$$

where $\bar{\eta}_{ijpq}$ is the anisotropic viscosity tensor (unit is Pa s$^{1/n}$) and $II_{\dot{\varepsilon}}$ is the second invariant of strain rate. I choose the second invariant of strain rate rather than stress because strain rate is known for most of the experimental setup and stress is the unknown variable. With an abbreviated (Voigt) notation, this equation becomes

$$\sigma_i = 2\bar{\eta}_{ij} II_{\dot{\varepsilon}}^{1-n/2n} \dot{\varepsilon}_j \quad (\text{Voigt notation}). \tag{A2}$$

Let us examine how the viscosity matrix, $\bar{\eta}_{ijpq}$ (or $\bar{\eta}_{ij}$ in the Voigt notation), is related to the flow laws of various slip systems. To do this, I assume that the viscosity tensor is written in the crystal reference frame. For crystals with orthotropic symmetry (cubic, tetragonal, hexagonal, and orthorhombic), Eq. (A2) is given by

$$\begin{pmatrix} \sigma_1'' \\ \sigma_2'' \\ \sigma_3'' \\ \sigma_4'' \\ \sigma_5'' \\ \sigma_6'' \end{pmatrix} = 2II_{\dot{\varepsilon}''}^{1-n/2n} \begin{pmatrix} \bar{\eta}_{11}'' & \bar{\eta}_{12}'' & \bar{\eta}_{13}'' & 0 & 0 & 0 \\ \bar{\eta}_{12}'' & \bar{\eta}_{22}'' & \bar{\eta}_{23}'' & 0 & 0 & 0 \\ \bar{\eta}_{13}'' & \bar{\eta}_{23}'' & \bar{\eta}_{33}'' & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{\eta}_{44}'' & 0 & 0 \\ 0 & 0 & 0 & 0 & \bar{\eta}_{55}'' & 0 \\ 0 & 0 & 0 & 0 & 0 & \bar{\eta}_{66}'' \end{pmatrix} \times \begin{pmatrix} \dot{\varepsilon}_1'' \\ \dot{\varepsilon}_2'' \\ \dot{\varepsilon}_3'' \\ \dot{\varepsilon}_4'' \\ \dot{\varepsilon}_5'' \\ \dot{\varepsilon}_6'' \end{pmatrix}. \tag{A3}$$

Let us consider a cubic crystal such as MgO. MgO belongs to a B1-type structure (NaCl-type structure) in which two slip systems are identified: $\langle 110\rangle\{001\}$ and $\langle 110\rangle\{1\bar{1}0\}$. These two sets of slip systems provide five independent strain components so that a polycrystalline aggregate can deform homogeneously using these two slip systems. For a cubic system, there will be three independent viscosities, viz.,

$$\begin{pmatrix} \sigma_1'' \\ \sigma_2'' \\ \sigma_3'' \\ \sigma_4'' \\ \sigma_5'' \\ \sigma_6'' \end{pmatrix} = 2II_{\dot{\varepsilon}''}^{1-n/2n} \begin{pmatrix} \bar{\eta}_{11}'' & \bar{\eta}_{12}'' & \bar{\eta}_{12}'' & 0 & 0 & 0 \\ \bar{\eta}_{12}'' & \bar{\eta}_{11}'' & \bar{\eta}_{12}'' & 0 & 0 & 0 \\ \bar{\eta}_{12}'' & \bar{\eta}_{12}'' & \bar{\eta}_{11}'' & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{\eta}_{44}'' & 0 & 0 \\ 0 & 0 & 0 & 0 & \bar{\eta}_{44}'' & 0 \\ 0 & 0 & 0 & 0 & 0 & \bar{\eta}_{44}'' \end{pmatrix} \times \begin{pmatrix} \dot{\varepsilon}_1'' \\ \dot{\varepsilon}_2'' \\ \dot{\varepsilon}_3'' \\ \dot{\varepsilon}_4'' \\ \dot{\varepsilon}_5'' \\ \dot{\varepsilon}_6'' \end{pmatrix}. \quad \text{(A4)}$$

When one uses the fact that there is no volumetric strain for ductile deformation, this leads to a five-component expression of stress-strain rate relationship, viz.,

$$\begin{pmatrix} \frac{\sigma_1''-\sigma_2''}{2} \\ \frac{\sigma_2''-\sigma_3''}{2} \\ \sigma_4'' \\ \sigma_5'' \\ \sigma_6'' \end{pmatrix} = 2II_{\dot{\varepsilon}''}^{1-n/2n} \begin{pmatrix} \bar{\eta}_I'' & 0 & 0 & 0 & 0 \\ 0 & \bar{\eta}_I'' & 0 & 0 & 0 \\ 0 & 0 & \bar{\eta}_{II}'' & 0 & 0 \\ 0 & 0 & 0 & \bar{\eta}_{II}'' & 0 \\ 0 & 0 & 0 & 0 & \bar{\eta}_{II}'' \end{pmatrix} \begin{pmatrix} \dot{\varepsilon}_1'' - \dot{\varepsilon}_2'' \\ \dot{\varepsilon}_2'' - \dot{\varepsilon}_3'' \\ \dot{\varepsilon}_4'' \\ \dot{\varepsilon}_5'' \\ \dot{\varepsilon}_6'' \end{pmatrix} \quad \text{(A5)}$$

with $\bar{\eta}_I'' \equiv \frac{\bar{\eta}_{11}''-\bar{\eta}_{12}''}{2}$ and $\bar{\eta}_{II}'' \equiv \bar{\eta}_{44}''$. For a material with the B1 (NaCl) structure, $\bar{\eta}_I''$ represents the viscosity corresponding to the $\langle 110\rangle\{1\bar{1}0\}$ slip system, and $\bar{\eta}_{II}''$ (η_{2323}) to the $\langle 110\rangle\{001\}$ slip system. In MgO, $\bar{\eta}_{II}''$ is a high-T slip system and $\bar{\eta}_I''$ is a low-T slip system.[27] The viscosity coefficients corresponding to other slip systems such as $\langle 1\bar{1}0\rangle\{111\}$ can be written by a combination of $\bar{\eta}_I''$ and $\bar{\eta}_{II}''$.

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