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# TEXTURE DEVELOPMENT IN HALITE: COMPARISON OF TAYLOR MODEL AND SELF-CONSISTENT THEORY

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**Abstract**—Halite, NaCl, has a strongly anisotropic single crystal yield surface with one family of easy slip systems $\{110\}\langle 1\bar{1}0\rangle$ (with only two independent ones in the set) and two families, $\{100\}\langle 011\rangle$ and $\{111\}\langle 1\bar{1}0\rangle$ which are six times stronger at room temperature. It is therefore a good example to compare theories of texture development at large strain. There are, indeed, large differences between predictions of the Taylor theory, which assumes homogeneous strain, and results of the self-consistent theory, which gives more freedom to grains to deform. These are expressed not only in texture but also in such microstructural parameters as grain shapes and active slip systems. One feature of the self-consistent model is that grains in soft orientations deform at a faster rate than hard grains. We performed simulations under different conditions for axial extension, compression and for simple shear and compared them with the few experiments that are available.

**Résumé**—Le sel gemme, NaCl, présente une surface de plasticité fortement anisotrope pour les monocristaux, avec une famille peu active de systèmes de glissement $\{110\}\langle 1\bar{1}0\rangle$ (dont seulement deux indépendants), et deux familles, $\{100\}\langle 011\rangle$ et $\{111\}\langle 1\bar{1}0\rangle$ qui sont cinq fois plus actives à la température ambiante. Il constitue donc un bon exemple pour comparer les théories du développement des textures à forte déformation. Il y a, c'est vrai, de grandes différences entre les prévisions de la théorie de Taylor qui suppose une déformation homogène, et les résultats de la théorie cohérente qui laisse les grains plus libres de se déformer. Ces différences s'expriment non seulement dans la texture, mais aussi dans des paramètres microstructuraux tels que la forme des grains et les systèmes de glissement actifs. Une caractéristique de ce modèle cohérent est que les grains en orientations douces se déforment plus rapidement que les grains durs. Nous effectuons des simulations pour différentes conditions d'allongement, de compression et de cisaillement simple, et nous les comparons avec les quelques expériences dont nous disposons.

**Zusammenfassung**—Halit, NaCl, hat eine sehr anisotrope Fließoberfläche mit einer Familie leichter Gleitsysteme $\{110\}\langle 1\bar{1}0\rangle$ (nur zwei unabhängige Gleitsysteme pro Satz) und den etwa fünfmal schwerer zu aktivierenden Systemen $\{100\}\langle 011\rangle$ und $\{111\}\langle 1\bar{1}0\rangle$. An diesem guten Materialbeispiel können daher Theorien der Texturentwicklung bei großen Verformungen geprüft werden. Tatsächlich bestehen auch zwischen den Voraussagen der Taylor-Theorie, die homogene Scherung annimmt, und Ergebnissen der selbstkonsistenten Theorie, die den Körnern größere Freiheit der Verformung erlaubt, große Unterschiede. Diese Unterschiede finden ihren Niederschlag nicht nur in der Textur, sondern auch in den Parametern der Mikrostruktur, wie Kornform und aktive Gleitsysteme. Ein Merkmal der selbstkonsistenten Theorie ist, daß Körner in leichten Orientierungen sich mit größerer Rate verformen als harte Körner. Wir haben Simulationen unter verschiedenen Bedingungen der achsialen Dehnung, Stauchung und für einfache Scherung durchgeführt und diese mit den wenigen verfügbaren Experimenten verglichen.

## 1. INTRODUCTION

In recent years the Taylor theory [1] has been successfully applied to model plastic deformation in monomineralic rocks. Simulated textures for quartzites and limestones compare reasonably with those observed in deformation experiments [e.g. 2, 3]. However, there are deficiencies in Taylor's classical model: it assumes homogeneous strain and requires all crystals to deform at the same rate and therefore to undergo the same shape change as the polycrystal [Fig. 1(a)]. In contrast to cubic metals, minerals often display low symmetry and asymmetrically disposed slip systems with very different critical resolved shear stress (crss). This results in a strongly anisotropic single crystal yield surface. Some orientations are much stronger than others and therefore are likely to deform at a slower rate. For minerals such as olivine the situation is even worse. Due to a lack of a sufficient number of independent slip systems, the yield surface is not closed in deviatoric stress space. The result is that such crystals cannot deform homogeneously. Some of these difficulties can be alleviated within the Taylor framework by using so-called "relaxed constraints" theories [4–6] which rescind the rigorous conditions of homogeneity for some strain components. In addition to considerable anisotropy, slip systems in minerals have a much more significant

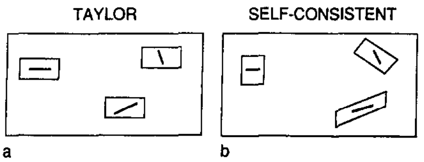

Fig. 1. Sketch contrasting Taylor (a) and self-consistent deformation (b).

rate dependence (stress exponent $n = 2$–$10$) than metals ($n = 50$–$100$). This has not been accounted for in the classical Taylor approach but may have a considerable influence on texture development [7]. A viscoplastic Taylor model in which vertices of the single crystal yield surface (SCYS) are effectively rounded has been used to select the activity on slip systems [8]. We are applying such a viscoplastic model. The influence of the rate dependence on texture is discussed in more detail elsewhere [9].

Other theories, such as those called collectively "self-consistent theories" (SC), may be more appropriate to model polycrystal plasticity in rate sensitive and strongly anisotropic materials. In this theory unfavorably oriented grains are allowed to deform less than favorably oriented grains [Fig. 1(b)]. We apply a viscoplastic SC approach to large deformations of halite (NaCl) and compare results with those from a viscoplastic Taylor theory. Halite has at low temperature a strongly anisotropic yield surface, and slip systems, including their rate and temperature dependence and work hardening characteristics, are well known which puts constraints on models. Our aim is to contrast results from the two theories and plausibly explain the differences. For lack of adequate experiments we are not in a position to give general recommendations about applicability but hope this presentation will stimulate experimentalists to pursue work on this system which is ideally suited to test different theories of polycrystal plasticity. It should be noted that both the SC and the Taylor theory model deformation by slip (dislocation glide) and are not applicable to recrystallization, diffusion or dissolution-reprecipitation mechanisms. In addition in our model we also neglect elasticity.

## 2. SELF-CONSISTENT VISCOPLASTIC DEFORMATION

Before presenting results of texture simulations in this system, it seems appropriate to describe briefly the basic principles of the self-consistent approach. (For details see [10]). For small deformations different self-consistent schemes were developed which take the interaction of each grain with the matrix environment into account [e.g. 11–14]. The environment is assumed to be an equivalent homogeneous medium.

Two extreme points of view have been used in plasticity theory. The first, developed by Taylor, requires complete strain compatibility between grains. This enforces a uniform plastic strain field throughout the polycrystal and sufficient slip systems to fulfill these conditions. These assumptions have been successful in modeling weakly anisotropic metals (e.g. f.c.c., b.c.c.), but creates difficulties for strongly anistropic systems. The second approach, developed by Sachs, imposes a constant stress direction in each grain, leading to a low number of active slip systems (predominantly single slip), but this theory has not been very successful, particularly for f.c.c. metals (e.g. [15]). The self-consistent schemes lie between these two extremes: they take account of both compatibility and equilibrium. The difference is illustrated in the schematic 2-dimensional SCYS in Fig. 2. For the Taylor condition deformation only occurs at a vertex, requiring high stresses. In Sachs a slip system is activated when the stress vector, which is assumed to be parallel to the externally applied stress direction, reaches the critical resolved shear stress. The SC condition is intermediate.

The model material is assumed to be both micro- and macroscopically viscoplastic; i.e. the plastic shear rate of each slip system is linked to the resolved shear stress acting in the system. Since elasticity is neglected the model is therefore restricted to large strains, with no significant path changes, and seems appropriate for large strain texture predictions in monotonic loadings like tension, compression or shear.

At the microscale, the shearing rate $\dot{\gamma}^s$ along a slip system $s$ is related to its resolved shear stress $\tau^s$ by a viscoplastic law. Here, the power law is used, i.e.

$$\frac{\dot{\gamma}^s}{\dot{\gamma}_0} = \left(\frac{\tau^s}{\tau_0^s}\right)^n \tag{1}$$

where $n$ is the stress exponent (the inverse of $m$, the strain-rate sensitivity factor), and $\dot{\gamma}_0$ and $\tau_0$ are the reference shearing rate and the reference crss, respectively. Microscopic hardening is considered to act through the latter term. The single crystal strain rate can be calculated by the formula

$$\mathbf{D}_{ij} = \sum_s \mathbf{R}^s_{ij}\left(\frac{\mathbf{R}^s_{kl}\mathbf{S}_{kl}}{\tau_0^s}\right)^n \tag{2}$$

where **D** and **S** are, respectively, the strain rate and deviatoric stress tensors (the summation convention

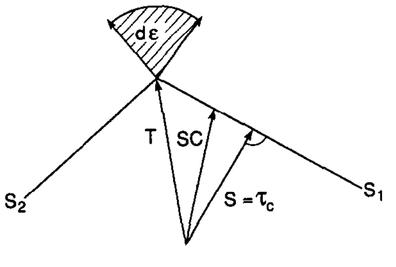

Fig. 2. Schematic two-dimensional single crystal yield surface to illustrate difference between Sachs (S), Taylor (T), and self-consistent (SC) model.